

result in loss of user privileges and other penalties.

\*\*\*\*\* STN Columbus \*\*\*\*\*

FILE 'HOME' ENTERED AT 14:30:34 ON 21 JUN 2006

=> fil casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CASREACT' ENTERED AT 14:30:42 ON 21 JUN 2006

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

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FILE CONTENT:1840 - 18 Jun 2006 VOL 144 ISS 25

New CAS Information Use Policies, enter HELP USAGETERMS for details.

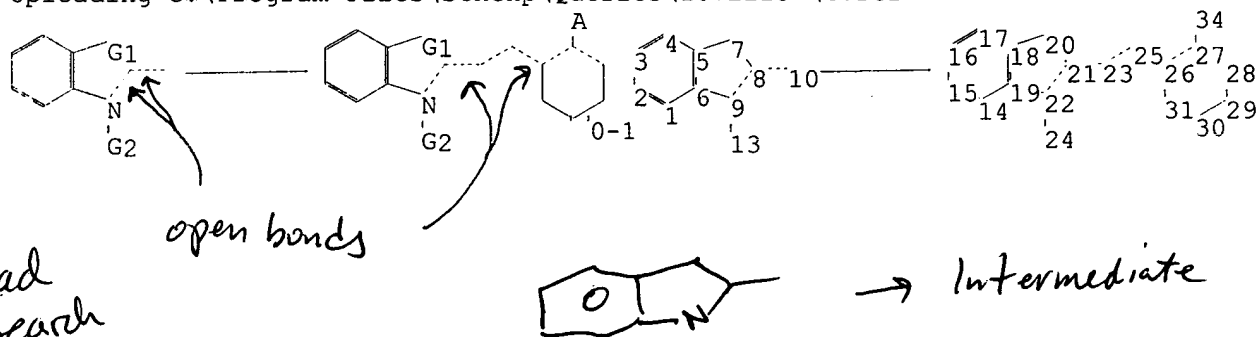
\*\*\*\*\*  
\*  
\* CASREACT now has more than 10 million reactions \*  
\*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Program Files\Stnexp\Queries\10722257\4.str



chain nodes :

10 13 23 24 25 34

ring nodes :

1 2 3 4 5 6 7 8 9 14 15 16 17 18 19 20 21 22 26 27 28 29 30 31

chain bonds :

8-10 9-13 21-23 22-24 23-25 25-26 27-34

ring bonds :

10/722,257

06/21/2006

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 14-15 14-19 15-16 16-17 17-18  
18-19 18-20 19-22 20-21 21-22 26-27 26-31 27-28 28-29 29-30 30-31

exact/norm bonds :

5-7 6-9 7-8 8-9 8-10 9-13 18-20 19-22 20-21 21-22 21-23 22-24 23-25  
25-26 26-27 26-31 27-28 27-34 28-29 29-30 30-31

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 14-15 14-19 15-16 16-17 17-18 18-19

G1:C,O,S,N

G2:Cb,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom  
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom 29:CLASS 30:Atom  
31:Atom 34:CLASS

fragments assigned product role:

containing 14

fragments assigned reactant/reagent role:

containing 1

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 14:31:10 FILE 'CASREACT'

SCREENING COMPLETE - 7209 REACTIONS TO VERIFY FROM

932 DOCUMENTS

100.0% DONE 7209 VERIFIED 320 HIT RXNS  
SEARCH TIME: 00.00.01

45 DOCS

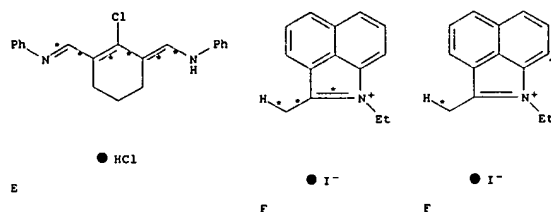
L2 45 SEA SSS FUL L1 ( 320 REACTIONS)

=> d ibib abs hit 1-45

L2 ANSWER 1 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 144:151804 CASREACT  
 TITLE: Novel synthetic route to pH-sensitive  
 2,6-bis(substituted  
 ethylidene)cyclohexanone/hydroxycy  
 anine dyes that absorb in the visible/near-infrared  
 regions  
 AUTHOR(S):  
 Martial;  
 CORPORATE SOURCE: Lee, Hyeran; Gupta, Rajni; Hojjat, Maryam  
 Department of Chemistry, Georgia State University,  
 Atlanta, GA, 30302, USA  
 SOURCE: Heterocyclic Communications (2005), 11(2), 129-134  
 CODEN: HCOMEX; ISSN: 0793-0283  
 PUBLISHER: Freund Publishing House Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Succinimide N-oxide anion-mediated reaction of heptamethine cyanines that  
 are chloro-substituted at the central position of the heptamethine moiety  
 furnishes the title dyes in high yield (80-96%). The ketones absorb in  
 the visible region, and upon protonation (pH<6) they are transformed into  
 hydroxycyanines that show an intense absorption in the near-IR region  
 (>700 nm).

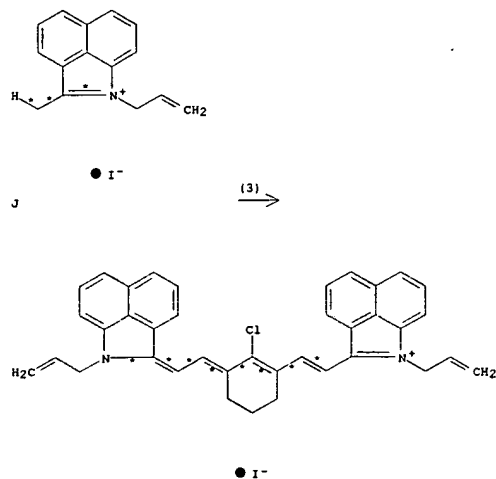
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(2) OF 15 E + 2 F ==> G...



(2) →

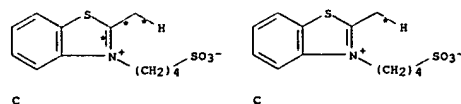
L2 ANSWER 1 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



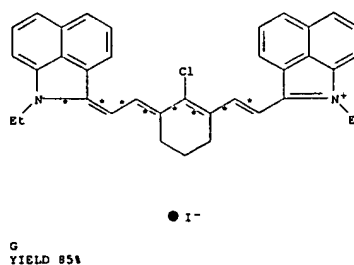
K  
 YIELD 80%

RX(3) RCT E 63857-00-1, J 134370-77-7  
 RGT H 141-78-6 AcOEt  
 PRO K 874201-52-2  
 SOL 64-17-5 EtOH  
 CON 5 hours, 80 deg C

RX(4) OF 15 ... 2 C + E ==> L...

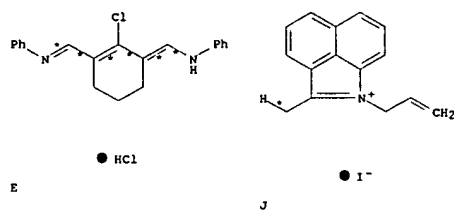


L2 ANSWER 1 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(2) RCT E 63857-00-1, F 5529-78-2  
 RGT H 141-78-6 AcOEt  
 PRO G 874201-50-0  
 SOL 64-17-5 EtOH  
 CON 5 hours, 80 deg C

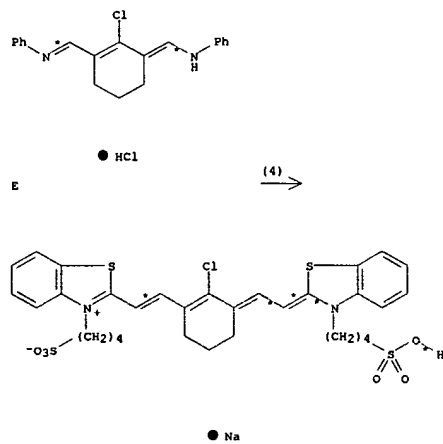
RX(3) OF 15 E + 2 J ==> K...



E

J

L2 ANSWER 1 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

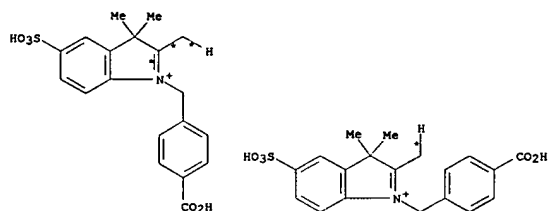


L  
 YIELD 84%

RX(4) RCT C 55526-95-9, E 63857-00-1  
 RGT H 141-78-6 AcOEt  
 PRO L 874201-54-4  
 SOL 64-17-5 EtOH  
 CON 5 hours, 80 deg C

L2 ANSWER 2 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 143:366898 CASREACT  
 TITLE: Novel heptamethine 3H-indocyanines and their spectral properties  
 AUTHOR(S): Wang, Li Qiu; Peng, Xiao Jun; Lu, Er Hu; Cui, Jing Nan; Gao, Xin Qin  
 CORPORATE SOURCE: State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian, 116012, Peop. Rep. China  
 SOURCE: Chinese Chemical Letters (2005), 16(4), 461-464  
 CODEN: CCLEET; ISSN: 1001-8417  
 PUBLISHER: Chinese Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Novel heptamethine 3H-indocyanine dyes are synthesized and embedded into a matrix of silica gel derived from tetraethoxysilicate. The photophys. properties of these near IR dyes in various solvents and in SiO2 sol gel were studied. The dyes containing cyclohexenylene bridge and N-(p-carboxy)benzyl groups have better photostability and longer absorption wavelength than those containing linear heptamethine bridge and/or N-(5-carboxy)pentanyl groups. The absorption maxima of these dyes are in reverse proportion to the polarity of the solvents. The microenvironment of the dyes in SiO2 sol-gel characters medium polarity (between methanol and DMF) according to the absorption maxima.  
 REFERENCE COUNT: 6  
 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

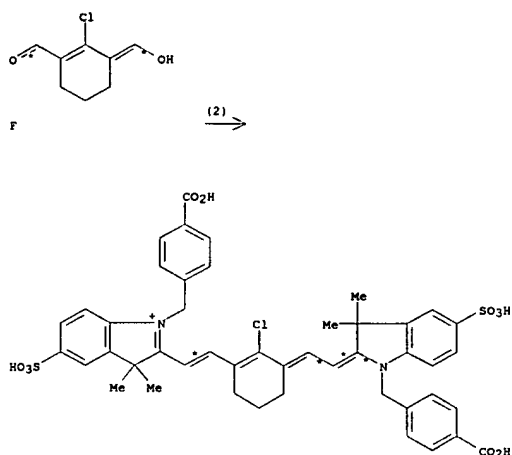
RX(2) OF 4 2 A + F ==> G



A

A

L2 ANSWER 2 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

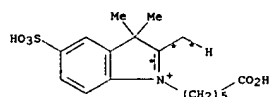


G

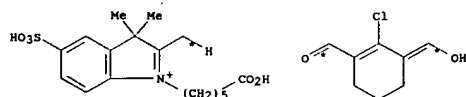
RX(2) RCT A 732241-24-6, F 61010-04-6  
 RGT D 108-24-7 Ac2O  
 PRO G 866364-73-0  
 SOL 75-07-0 MeCHO  
 CON room temperature

RX(3) OF 4 2 I + F ==> J

L2 ANSWER 2 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



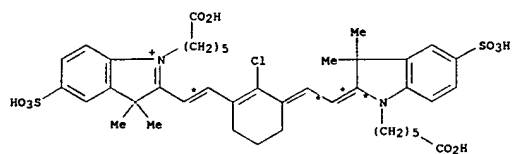
I



I



F

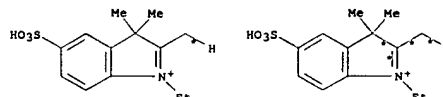


J

RX(3) RCT I 749838-12-0, F 61010-04-6  
 RGT D 108-24-7 Ac2O  
 PRO J 866364-74-1  
 SOL 75-07-0 MeCHO  
 CON room temperature

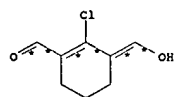
RX(4) OF 4 2 K + F ==> L

L2 ANSWER 2 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

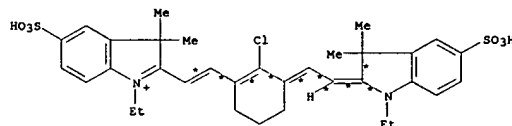


K

K



F

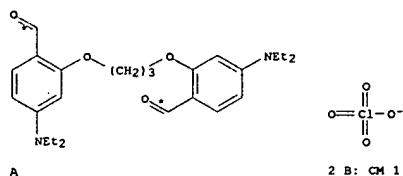


L

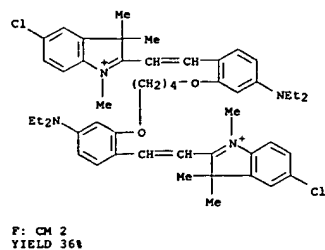
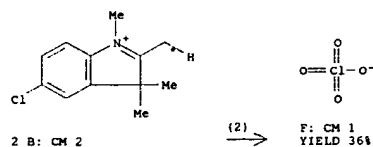
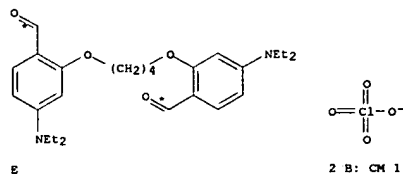
RX(4) RCT K 769919-84-0, F 61010-04-6  
 RGT D 108-24-7 Ac2O  
 PRO L 866364-75-2  
 SOL 75-07-0 MeCHO  
 CON room temperature

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 143:327738 CASREACT  
 TITLE: Synthesis and optical recording properties of coupled hemicyanine salts for DVD-R  
 AUTHOR(S): Lee, Chul Joo; Min, Kyung Sun; Park, Ki Hong  
 CORPORATE SOURCE: Optoelectronic Materials Research Center, Korea Institute of Science and Technology, Seoul, 136-791, S. Korea  
 SOURCE: Journal of Photochemistry (2003), 10(2), 209-214  
 CODEN: JOPHFS; ISSN: 1225-8555  
 PUBLISHER: Korean Society of Photochemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Seven coupled hemicyanine dyes with tri- to pentamethylenedioxy spacers were successfully synthesized by condensation of alkylendioxy-coupled dialdehydes with 2 different indoline perchlorates. These coupled dyes had better thermal properties (high decomposition temperature, stiff decomposition behavior) and higher molar absorption properties than an uncoupled dye. The coupled dyes with perchlorate anions showed strong exothermic decomposition while those with hexafluorophosphate anions showed endothermic decomposition. As the methylene coupling length increased, thermal properties decreased and dyes with even-numbered spacers were more thermally stable than dyes with odd spacers. Two dyes exhibited the best recording properties with the lowest jitter value of 7.5.apprx.9.5% in authorizing disks.  
 REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(1) OF 34 ...A + 2 B ==> C



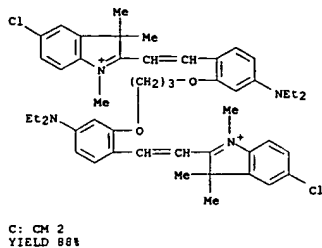
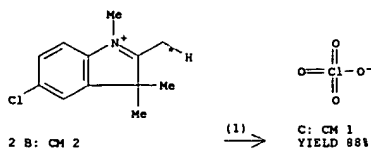
L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(2) RCT E 514813-62-8, B 31878-25-8  
 PRO F 514813-74-2  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

RX(3) OF 34 ...G + 2 B ==> H

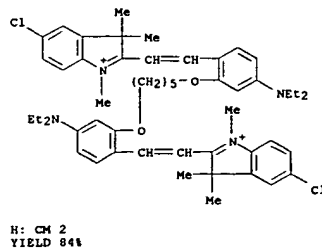
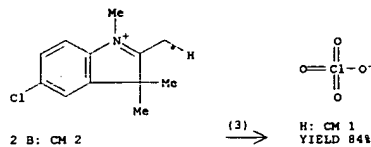
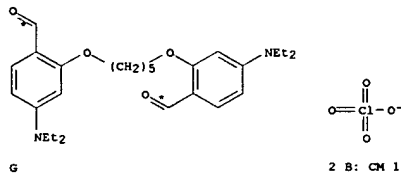
L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(1) RCT A 514813-61-7, B 31878-25-8  
 PRO C 514813-72-0  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

RX(2) OF 34 ...E + 2 B ==> F

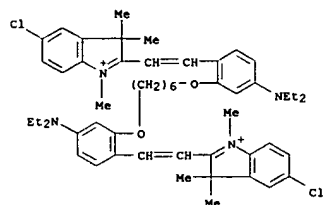
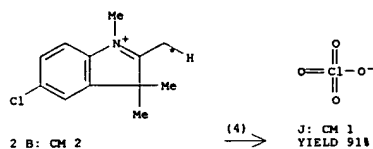
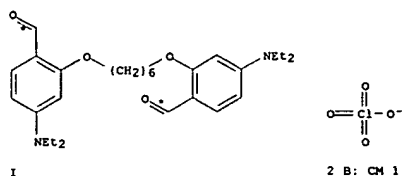
L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(3) RCT G 514813-63-9, B 31878-25-8  
 PRO H 514813-76-4  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

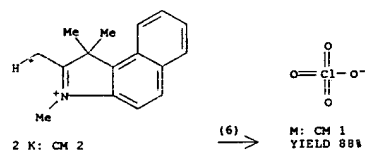
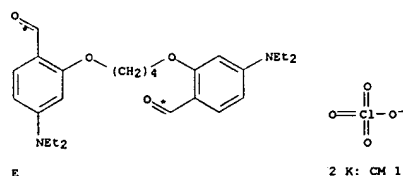
RX(4) OF 34 ...I + 2 B ==> J

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

J: CH 1  
YIELD 91%

RX(4) RCT I 514813-65-1, B 31878-25-8  
PRO J 514813-78-6  
SOL 64-17-5 EtOH  
CON 3 days, reflux

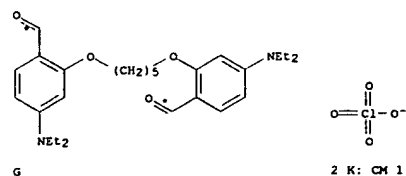
L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

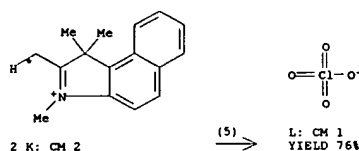
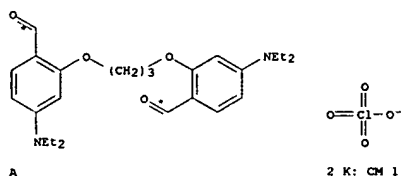
RX(6) RCT E 514813-62-8, K 92570-02-0  
PRO M 514813-93-5  
SOL 64-17-5 EtOH  
CON 3 days, reflux

RX(7) OF 34 ...G + 2 K ==&gt; N



L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(5) OF 34 ...A + 2 K ==&gt; L

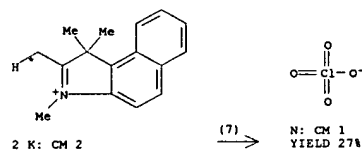


\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT A 514813-61-7, K 92570-02-0  
PRO L 514813-92-4  
SOL 64-17-5 EtOH  
CON 3 days, reflux

RX(6) OF 34 ...E + 2 K ==&gt; M

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

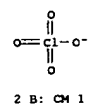
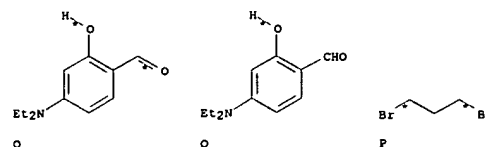


\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

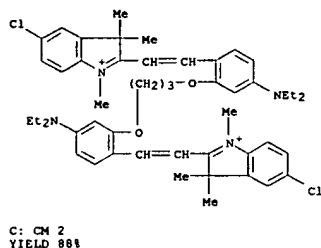
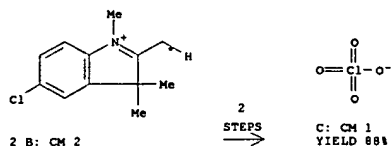
RX(7) RCT G 514813-63-9, K 92570-02-0  
PRO N 514813-94-6  
SOL 64-17-5 EtOH  
CON 3 days, reflux

RX(14) OF 34 COMPOSED OF RX(8), RX(1)

RX(14) 2 O + P + 2 B ==&gt; C



L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(8) RCT O 17754-90-4

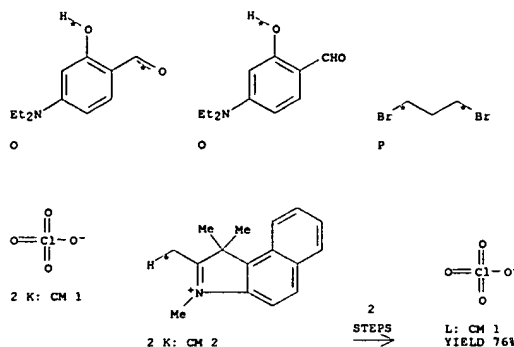
STAGE(1)  
RGT Q 1310-58-3 KOH  
SOL 109-99-9 THF  
CON 100 deg C

STAGE(2)  
RCT P 109-64-8  
CON 24 hours, reflux

PRO A 514813-61-7  
NTE Aliquat 336 used

RX(1) RCT A 514813-61-7, B 31878-25-8  
PRO C 514813-72-0  
SOL 64-17-5 EtOH  
CON 3 days, reflux

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(8) RCT O 17754-90-4

STAGE(1)  
RGT Q 1310-58-3 KOH  
SOL 109-99-9 THF  
CON 100 deg C

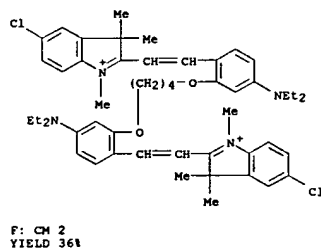
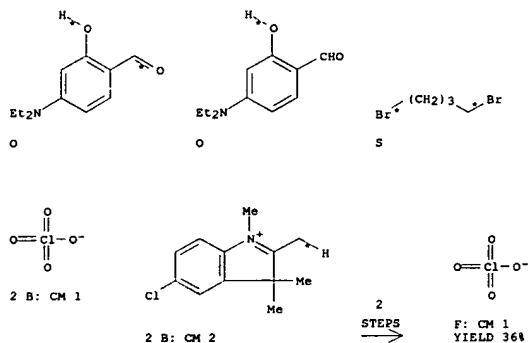
STAGE(2)  
RCT P 109-64-8  
CON 24 hours, reflux

PRO A 514813-61-7  
NTE Aliquat 336 used

RX(5) RCT A 514813-61-7, K 92570-02-0  
PRO L 514813-92-4  
SOL 64-17-5 EtOH  
CON 3 days, reflux

RX(16) OF 34 COMPOSED OF RX(9), RX(2)  
RX(16) 2 O + S + 2 B ==> F

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(9) RCT O 17754-90-4

STAGE(1)  
RGT Q 1310-58-3 KOH  
SOL 109-99-9 THF  
CON 100 deg C

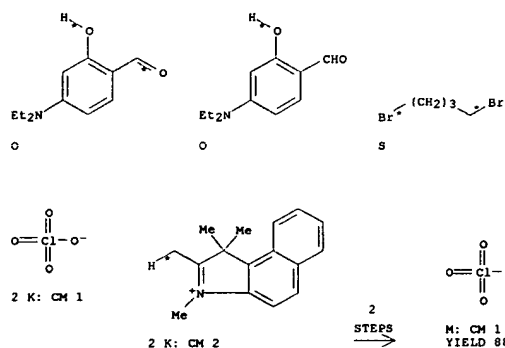
STAGE(2)  
RCT S 110-52-1  
CON 24 hours, reflux

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO E 514813-62-8  
NTE Aliquat 336 used

RX(2) RCT E 514813-62-8, B 31878-25-8  
PRO F 514813-74-2  
SOL 64-17-5 EtOH  
CON 3 days, reflux

RX(17) OF 34 COMPOSED OF RX(9), RX(6)  
RX(17) 2 O + S + 2 K ==> M



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(9) RCT O 17754-90-4

STAGE(1)  
RGT Q 1310-58-3 KOH  
SOL 109-99-9 THF  
CON 100 deg C

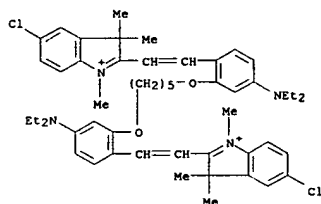
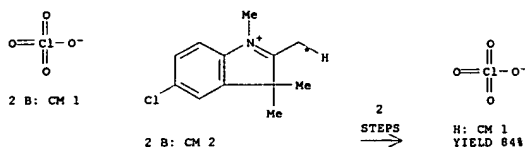
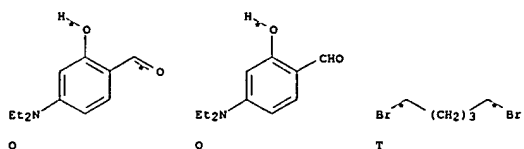
STAGE(2)  
RCT S 110-52-1  
CON 24 hours, reflux

PRO E 514813-62-8  
NTE Aliquat 336 used

RX(6) RCT E 514813-62-8, K 92570-02-0  
PRO M 514813-93-5

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

RX(18) OF 34 COMPOSED OF RX(10), RX(3)  
 RX(18) 2 O + T + 2 B ==> H



H: CM 2  
 YIELD 84%

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 RX(10) RCT O 17754-90-4

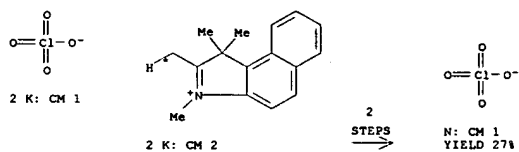
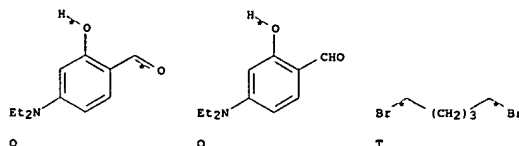
STAGE(1)  
 RGT Q 1310-58-3 KOH  
 SOL 109-99-9 THF  
 CON 100 deg C

STAGE(2)  
 RCT T 111-24-0  
 CON 24 hours, reflux

PRO G 514813-63-9  
 NTE Aliquat 336 used

RX(3) RCT G 514813-63-9, B 31878-25-8  
 PRO H 514813-76-4  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

RX(19) OF 34 COMPOSED OF RX(10), RX(7)  
 RX(19) 2 O + T + 2 K ==> N



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(10) RCT O 17754-90-4

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

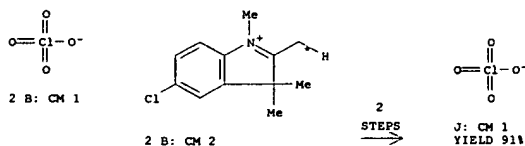
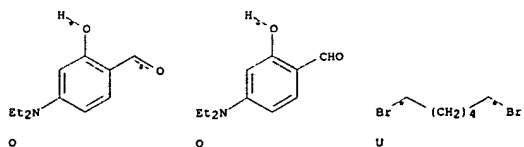
STAGE(1)  
 RGT Q 1310-58-3 KOH  
 SOL 109-99-9 THF  
 CON 100 deg C

STAGE(2)  
 RCT T 111-24-0  
 CON 24 hours, reflux

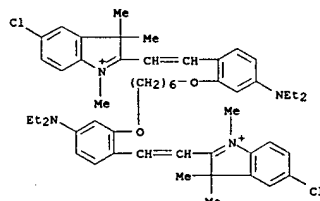
PRO G 514813-63-9  
 NTE Aliquat 336 used

RX(7) RCT G 514813-63-9, K 92570-02-0  
 PRO N 514813-94-6  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

RX(20) OF 34 COMPOSED OF RX(11), RX(4)  
 RX(20) 2 O + U + 2 B ==> J



L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



J: CM 2  
 YIELD 91%

RX(11) RCT O 17754-90-4

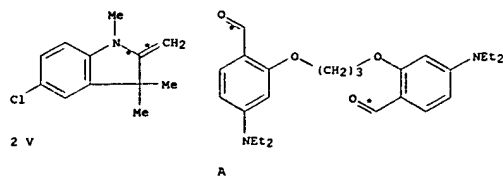
STAGE(1)  
 RGT Q 1310-58-3 KOH  
 SOL 109-99-9 THF  
 CON 100 deg C

STAGE(2)  
 RCT U 629-03-8  
 CON 24 hours, reflux

PRO I 514813-65-1  
 NTE Aliquat 336 used

RX(4) RCT I 514813-65-1, B 31878-25-8  
 PRO J 514813-78-6  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

RX(21) OF 34 COMPOSED OF RX(12), RX(1)  
 RX(21) 2 V + A ==> C

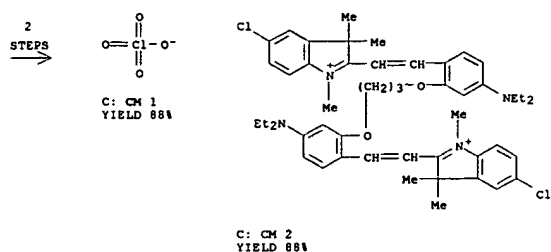


2 V

A



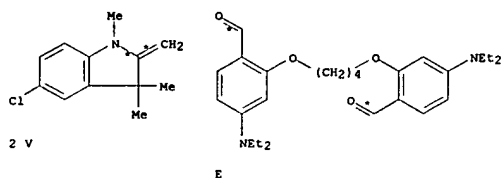
L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



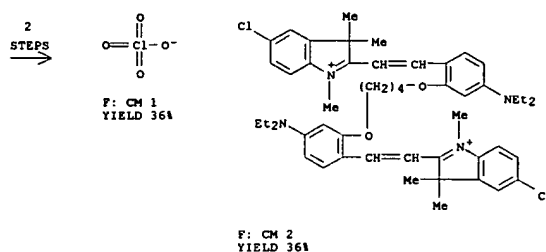
RX(12) RCT V 6872-17-9  
RGT W 7601-90-3 HClO4  
PRO B 31878-25-8  
SOL 7732-18-5 Water, 60-29-7 Et2O  
CON 5 hours, room temperature

RX(1) RCT A 514813-61-7, B 31878-25-8  
PRO C 514813-72-0  
SOL 64-17-5 EtOH  
CON 3 days, reflux

RX(22) OF 34 COMPOSED OF RX(12), RX(2)  
RX(22) 2 V + E → F



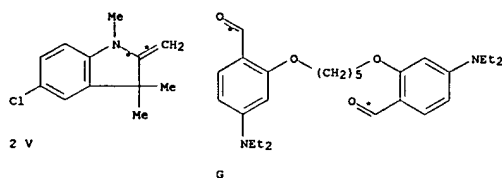
L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



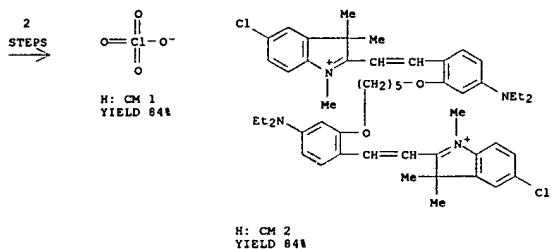
RX(12) RCT V 6872-17-9  
RGT W 7601-90-3 HClO4  
PRO B 31878-25-8  
SOL 7732-18-5 Water, 60-29-7 Et2O  
CON 5 hours, room temperature

RX(2) RCT E 514813-62-8, B 31878-25-8  
PRO F 514813-74-2  
SOL 64-17-5 EtOH  
CON 3 days, reflux

RX(23) OF 34 COMPOSED OF RX(12), RX(3)  
RX(23) 2 V + G → H



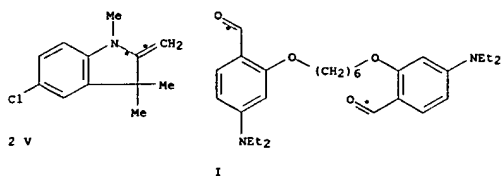
L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



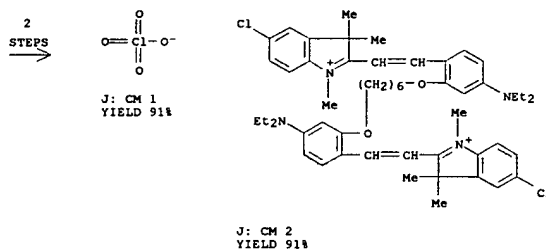
RX(12) RCT V 6872-17-9  
RGT W 7601-90-3 HClO4  
PRO B 31878-25-8  
SOL 7732-18-5 Water, 60-29-7 Et2O  
CON 5 hours, room temperature

RX(3) RCT G 514813-63-9, B 31878-25-8  
PRO H 514813-76-4  
SOL 64-17-5 EtOH  
CON 3 days, reflux

RX(24) OF 34 COMPOSED OF RX(12), RX(4)  
RX(24) 2 V + I → J



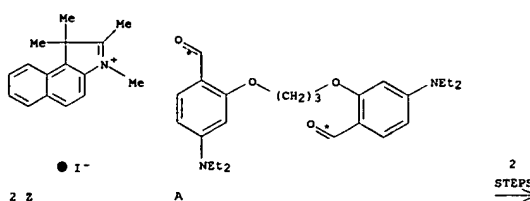
L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(12) RCT V 6872-17-9  
RGT W 7601-90-3 HClO4  
PRO B 31878-25-8  
SOL 7732-18-5 Water, 60-29-7 Et2O  
CON 5 hours, room temperature

RX(4) RCT I 514813-65-1, B 31878-25-8  
PRO J 514813-78-6  
SOL 64-17-5 EtOH  
CON 3 days, reflux

RX(25) OF 34 COMPOSED OF RX(13), RX(5)  
RX(25) 2 Z + A → L



L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

L: CM 1  
YIELD 76%

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(13) RCT Z 58464-25-8

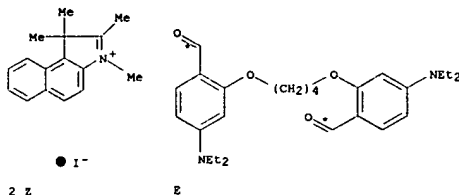
## STAGE(1)

RGT AA 1310-73-2 NaOH  
SOL 67-56-1 MeOH  
CON 2 hours, room temperature

## STAGE(2)

RGT W 7601-90-3 HClO4  
SOL 7732-18-5 Water

PRO K 92570-02-0

RX(5) RCT A 514813-61-7, K 92570-02-0  
PRO L 514813-92-4  
SOL 64-17-5 EtOH  
CON 3 days, refluxRX(26) OF 34 COMPOSED OF RX(13), RX(6)  
RX(26) 2 Z + E ==> M

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

M: CM 1  
YIELD 88%

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(13) RCT Z 58464-25-8

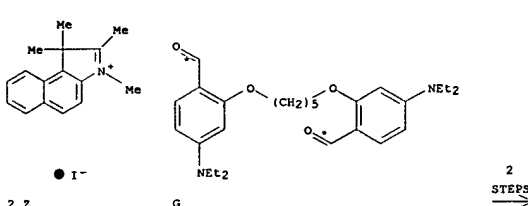
## STAGE(1)

RGT AA 1310-73-2 NaOH  
SOL 67-56-1 MeOH  
CON 2 hours, room temperature

## STAGE(2)

RGT W 7601-90-3 HClO4  
SOL 7732-18-5 Water

PRO K 92570-02-0

RX(6) RCT E 514813-62-8, K 92570-02-0  
PRO M 514813-93-5  
SOL 64-17-5 EtOH  
CON 3 days, refluxRX(27) OF 34 COMPOSED OF RX(13), RX(7)  
RX(27) 2 Z + G ==> M

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

N: CM 1  
YIELD 27%

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(13) RCT Z 58464-25-8

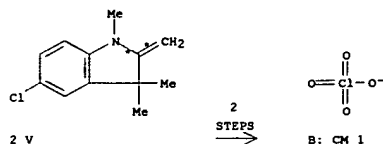
## STAGE(1)

RGT AA 1310-73-2 NaOH  
SOL 67-56-1 MeOH  
CON 2 hours, room temperature

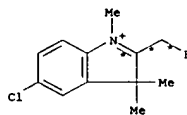
## STAGE(2)

RGT W 7601-90-3 HClO4  
SOL 7732-18-5 Water

PRO K 92570-02-0

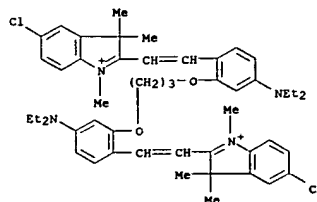
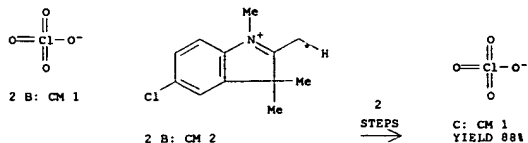
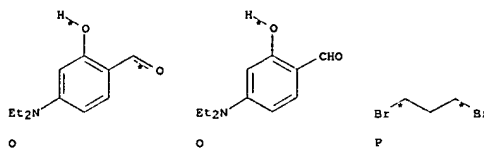
RX(7) RCT G 514813-63-9, K 92570-02-0  
PRO N 514813-94-6  
SOL 64-17-5 EtOH  
CON 3 days, refluxRX(28) OF 34 COMPOSED OF REACTION SEQUENCE RX(12), RX(1)  
AND REACTION SEQUENCE RX(8), RX(1)  
...2 V ==> B...  
...2 O + P + 2 B ==> C

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



B: CM 2

START NEXT REACTION SEQUENCE

C: CM 2  
YIELD 88%

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(12) RCT V 6872-17-9  
 RGT W 7601-90-3 HClO4  
 PRO B 31878-25-8  
 SOL 7732-18-5 Water, 60-29-7 Et2O  
 CON 5 hours, room temperature

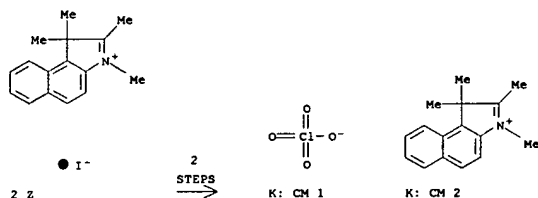
RX(8) RCT O 17754-90-4  
 STAGE(1)  
 RGT Q 1310-58-3 KOH  
 SOL 109-99-9 THF  
 CON 100 deg C

STAGE(2)  
 RCT P 109-64-8  
 CON 24 hours, reflux

PRO A 514813-61-7  
 NTE Aliquat 336 used

RX(1) RCT A 514813-61-7, B 31878-25-8  
 PRO C 514813-72-0  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

RX(29) OF 34 COMPOSED OF REACTION SEQUENCE RX(13), RX(5)  
 AND REACTION SEQUENCE RX(8), RX(5)  
 ...2 Z ==> K...  
 ...2 O + P + 2 K ==> L



START NEXT REACTION SEQUENCE

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

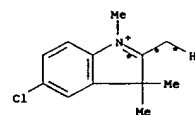
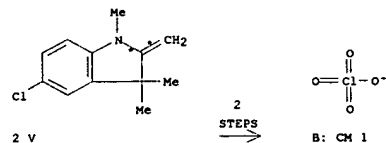
STAGE(1)  
 RGT Q 1310-58-3 KOH  
 SOL 109-99-9 THF  
 CON 100 deg C

STAGE(2)  
 RCT P 109-64-8  
 CON 24 hours, reflux

PRO A 514813-61-7  
 NTE Aliquat 336 used

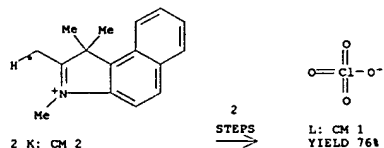
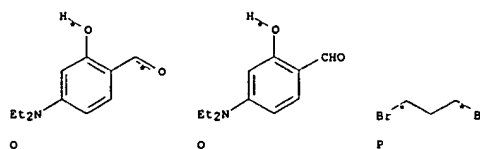
RX(5) RCT A 514813-61-7, K 92570-02-0  
 PRO L 514813-92-4  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

RX(30) OF 34 COMPOSED OF REACTION SEQUENCE RX(12), RX(2)  
 AND REACTION SEQUENCE RX(9), RX(2)  
 ...2 V ==> B...  
 ...2 O + S + 2 B ==> F



START NEXT REACTION SEQUENCE

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(13) RCT Z 58464-25-8

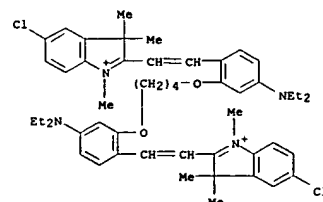
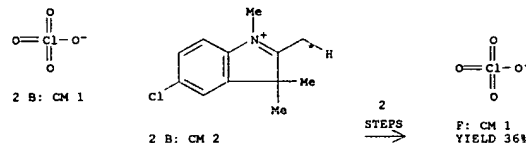
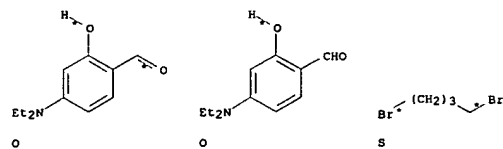
STAGE(1)  
 RGT AA 1310-73-2 NaOH  
 SOL 67-56-1 MeOH  
 CON 2 hours, room temperature

STAGE(2)  
 RGT W 7601-90-3 HClO4  
 SOL 7732-18-5 Water

PRO K 92570-02-0

RX(8) RCT O 17754-90-4

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



F: CM 2  
YIELD 36%

RX(12) RCT V 6872-17-9  
 RGT W 7601-90-3 HClO4  
 PRO B 31878-25-8  
 SOL 7732-18-5 Water, 60-29-7 Et2O  
 CON 5 hours, room temperature

RX(9) RCT O 17754-90-4

STAGE(1)  
 RGT Q 1310-58-3 KOH

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 SOL 109-99-9 THF  
 CON 100 deg C

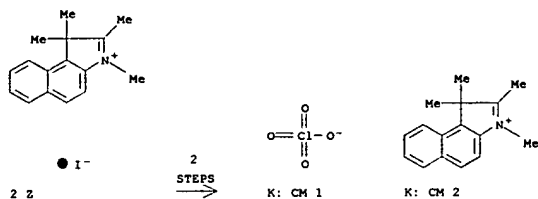
STAGE(2)  
 RCT S 110-52-1  
 CON 24 hours, reflux

PRO E 514813-62-8  
 NTE Aliquot 336 used

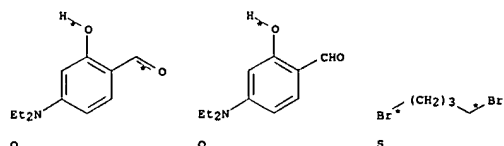
RX(2) RCT E 514813-62-8, B 31878-25-8  
 PRO F 514813-74-2  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

RX(31) OF 34 COMPOSED OF REACTION SEQUENCE RX(13), RX(6)  
 AND REACTION SEQUENCE RX(9), RX(6)

...2 Z ==> K...  
 ...2 O + S + 2 K ==> M



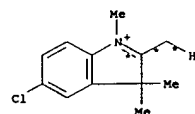
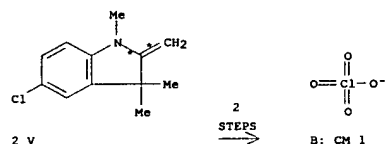
START NEXT REACTION SEQUENCE



L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 PRO M 514813-93-5  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

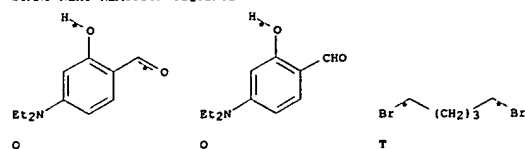
RX(32) OF 34 COMPOSED OF REACTION SEQUENCE RX(12), RX(3)  
 AND REACTION SEQUENCE RX(10), RX(3)

...2 V ==> B...  
 ...2 O + T + 2 B ==> H



B: CM 2

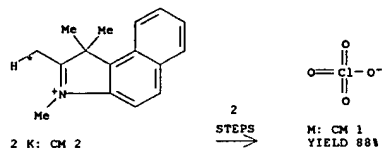
START NEXT REACTION SEQUENCE



L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



2 K: CM 1



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(13) RCT 2 58464-25-8

STAGE(1)  
 RGT AA 1310-73-2 NaOH  
 SOL 67-56-1 MeOH  
 CON 2 hours, room temperature

STAGE(2)  
 RGT W 7601-90-3 HClO4  
 SOL 7732-18-5 Water

PRO K 92570-02-0

RX(9) RCT O 17754-90-4

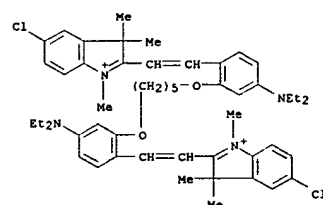
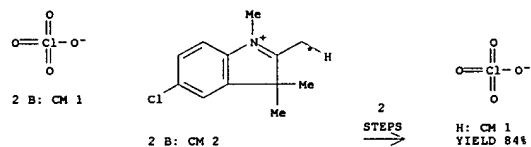
STAGE(1)  
 RGT Q 1310-58-3 KOH  
 SOL 109-99-9 THF  
 CON 100 deg C

STAGE(2)  
 RCT S 110-52-1  
 CON 24 hours, reflux

PRO E 514813-62-8  
 NTE Aliquot 336 used

RX(6) RCT E 514813-62-8, K 92570-02-0

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



H: CM 2  
 YIELD 84%

RX(12) RCT V 6872-17-9  
 RGT W 7601-90-3 HClO4  
 PRO B 31878-25-8  
 SOL 7732-18-5 Water, 60-29-7 Et2O  
 CON 5 hours, room temperature

RX(10) RCT O 17754-90-4

STAGE(1)  
 RGT Q 1310-58-3 KOH  
 SOL 109-99-9 THF  
 CON 100 deg C

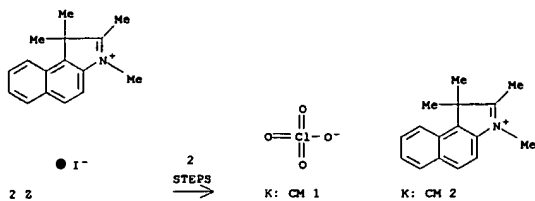
STAGE(2)  
 RCT T 111-24-0  
 CON 24 hours, reflux

PRO G 514813-63-9  
 NTE Aliquot 336 used

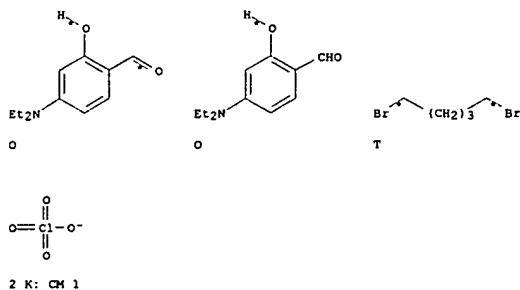
RX(3) RCT G 514813-63-9, B 31878-25-8  
 PRO H 514813-76-4  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

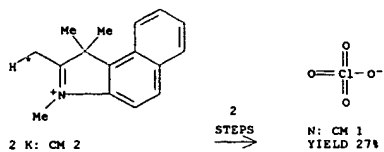
RX(33) OF 34 COMPOSED OF REACTION SEQUENCE RX(13), RX(7)  
 AND REACTION SEQUENCE RX(10), RX(7)  
 ...2 Z ==> K...  
 ...2 O + T + 2 K ==> N



START NEXT REACTION SEQUENCE



L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(13) RCT Z 58464-25-8

STAGE(1)

RGT AA 1310-73-2 NaOH  
 SOL 67-56-1 MeOH  
 CON 2 hours, room temperature

STAGE(2)

RGT W 7601-90-3 HClO<sub>4</sub>  
 SOL 7732-18-5 Water

PRO K 92570-02-0

RX(10) RCT O 17754-90-4

STAGE(1)

RGT Q 1310-58-3 KOH  
 SOL 109-99-9 THF  
 CON 100 deg C

STAGE(2)

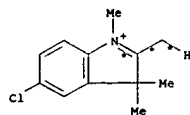
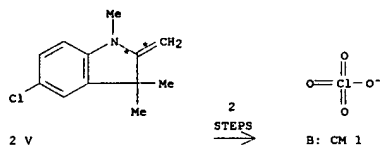
RCT T 111-24-0  
 CON 24 hours, reflux

PRO G 514813-63-9  
 NTE Aliquot 336 used

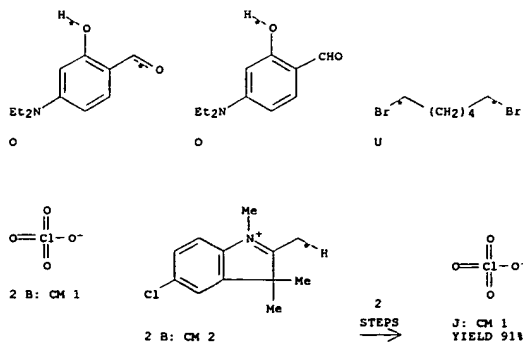
RX(7) RCT G 514813-63-9, K 92570-02-0  
 PRO N 514813-94-6  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

RX(34) OF 34 COMPOSED OF REACTION SEQUENCE RX(12), RX(4)  
 AND REACTION SEQUENCE RX(11), RX(4)  
 ...2 V ==> B...  
 ...2 O + U + 2 B ==> J

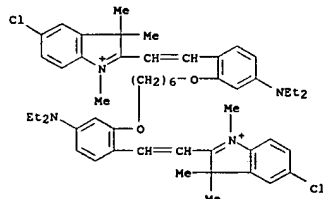
L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



START NEXT REACTION SEQUENCE



L2 ANSWER 3 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

J: CH 2  
YIELD 91%

RX(12) RCT V 6872-17-9  
 RGT W 7601-90-3 HClO<sub>4</sub>  
 PRO B 31878-25-8  
 SOL 7732-18-5 Water, 60-29-7 Et<sub>2</sub>O  
 CON 5 hours, room temperature

RX(11) RCT O 17754-90-4

STAGE(1)

RGT Q 1310-58-3 KOH  
 SOL 109-99-9 THF  
 CON 100 deg C

STAGE(2)

RCT U 629-03-8  
 CON 24 hours, reflux

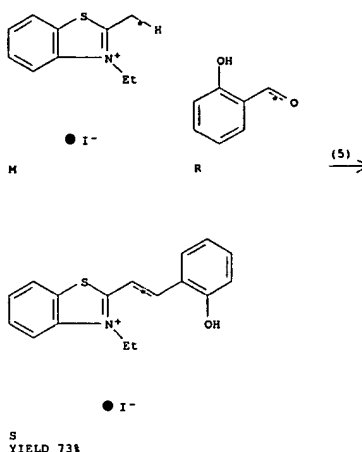
PRO I 514813-65-1  
 NTE Aliquot 336 used

RX(4) RCT I 514813-65-1, B 31878-25-8  
 PRO J 514813-70-6  
 SOL 64-17-5 EtOH  
 CON 3 days, reflux

L2 ANSWER 4 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 143:39891 CASREACT  
 TITLE: Novel Oxidative Self-Anchoring Fluorescent Substrates for the Histochemical Localization of Endogenous and Immunobound Peroxidase Activity  
 AUTHOR(S): Krieg, Reimar; Halbhuer, Karl-Juergen  
 CORPORATE SOURCE: Institute of Anatomy II, Friedrich Schiller University  
 SOURCE: Jena, Jena, D-07743, Germany  
 Journal of Molecular Histology (2004), 35(5), 471-487  
 CODEN: JMHQAO; ISSN: 1567-2379  
 PUBLISHER: Kluwer Academic Publishers  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Some 2-(2-styryl)-benzothiazole deriva. have been synthesized as novel fluorescent substrates for the localization of peroxidase activity. Excellent localization, high staining sensitivity and exceptionally low background staining were achieved by optimizing the choice of substrate. Multiple step-by-step anchoring of enzymically-activated individual substrate mols. to surrounding nucleophiles, related to the catalyzed reporter deposition (CARD) technique, is discussed. In contrast to tyramine conjugates, as employed in the CARD technique, the separation between reporting and anchoring function is eliminated, thus yielding a new fluorochrome with altered fluorescence properties after enzymic crosslinking. (E)-2-(2-[4-hydroxyphenyl] vinyl)-3-ethyl-1,3-benzothiazolium iodide has been found to the best substrate so far. This was demonstrated in histochem. applications for the localization of endogenous and immunobound peroxidase activity using fixed cryostat, paraffin or semi-thin Epon sections. The specific final reaction product is efficiently excitable over a wide spectrum from green to violet, providing an outstanding sensitive localization of sites of enzymic activity with high photo stability. In a comparative study with the Alexa Fluor 546-tyramine conjugate, endogenous and immunobound peroxidase activity was visualized and the results compared using an epi-fluorescence confocal laser scanning microscope. The novel substrate provided an improved specificity and very low background staining whereas the Alexa Fluor-tyramide exhibited a strong overall background staining. FITC-labeled secondary antibodies also yielded very low background staining but the staining was less specific compared with the biotin-based ABC amplification systems labeled with the selected substrate or the Alexa-tyramide. In conclusion, multiple fluorochrome generation close to sites of peroxidase activity, by enzymic crosslinking of styrene-related substrates, is a promising alternative to the fluorochrome-labeled tyramine ('tyramide') deposition technique.  
 REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(5) OF 21 M + R ==> S

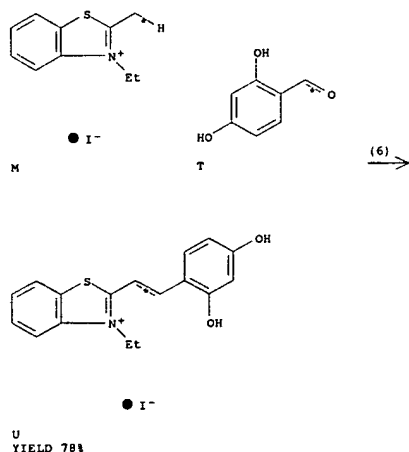
L2 ANSWER 4 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(5) RCT M 3119-93-5, R 90-02-6  
 PRO S 852335-82-1  
 CAT 110-89-4 Piperidine  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 60 minutes, reflux  
 SUBSTAGE(2) reflux -> -18 deg C  
 NTE stereoselective

RX(6) OF 21 M + T ==> U

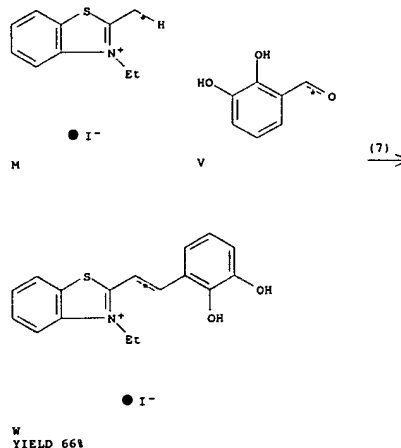
L2 ANSWER 4 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(6) RCT M 3119-93-5, T 95-01-2  
 PRO U 852335-83-2  
 CAT 110-89-4 Piperidine  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 60 minutes, reflux  
 SUBSTAGE(2) reflux -> -18 deg C  
 NTE stereoselective

RX(7) OF 21 M + V ==> W

L2 ANSWER 4 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

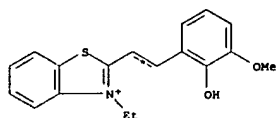
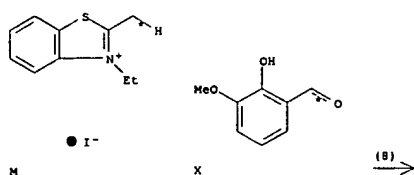


RX(7) RCT M 3119-93-5, V 24677-78-9  
 PRO W 852335-84-3  
 CAT 110-89-4 Piperidine  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 60 minutes, reflux  
 SUBSTAGE(2) reflux -> -18 deg C  
 NTE stereoselective

RX(8) OF 21 M + X ==> Y

L2 ANSWER 4 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



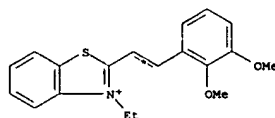
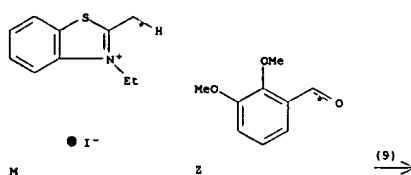
YIELD 93%

RX(8) RCT M 3119-93-5, X 148-53-8  
 PRO Y 852335-85-4  
 CAT 110-89-4 Piperidine  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 60 minutes, reflux  
 SUBSTAGE(2) reflux -> -18 deg C  
 NTE stereoselective

RX(9) OF 21 M + Z ==&gt; AA

L2 ANSWER 4 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



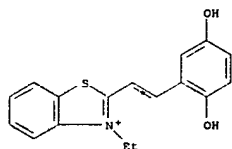
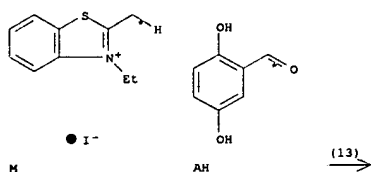
YIELD 66%

RX(9) RCT M 3119-93-5, Z 86-51-1  
 PRO AA 852335-86-5  
 CAT 110-89-4 Piperidine  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 60 minutes, reflux  
 SUBSTAGE(2) reflux -> -18 deg C  
 NTE stereoselective

RX(13) OF 21 M + AH ==&gt; AI

L2 ANSWER 4 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



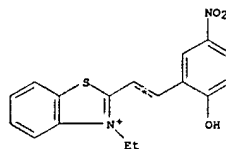
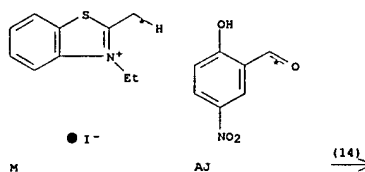
YIELD 40%

RX(13) RCT M 3119-93-5, AH 1194-98-5  
 PRO AI 852335-92-3  
 CAT 110-89-4 Piperidine  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 60 minutes, reflux  
 SUBSTAGE(2) reflux -> -18 deg C  
 NTE stereoselective

RX(14) OF 21 M + AJ ==&gt; AK

L2 ANSWER 4 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

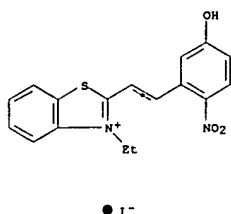
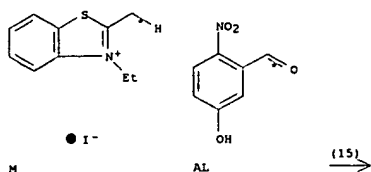


YIELD 95%

RX(14) RCT M 3119-93-5, AJ 97-51-8  
 PRO AK 852335-93-4  
 CAT 110-89-4 Piperidine  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 60 minutes, reflux  
 SUBSTAGE(2) reflux -> -18 deg C  
 NTE stereoselective

RX(15) OF 21 M + AL ==&gt; AM

L2 ANSWER 4 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

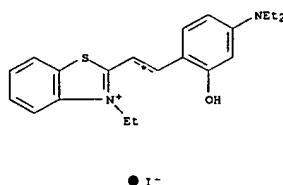
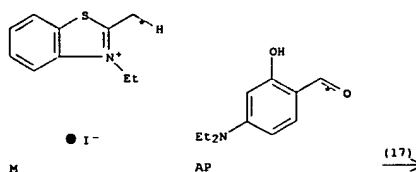


AM  
YIELD 72%

RX(15) RCT M 3119-93-5, AL 42454-06-8  
PRO AM 852335-94-5  
CAT 110-89-4 Piperidine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 60 minutes, reflux  
SUBSTAGE(2) reflux -> -18 deg C  
NTE stereoselective

RX(17) OF 21 M + AP ==> AQ

L2 ANSWER 4 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

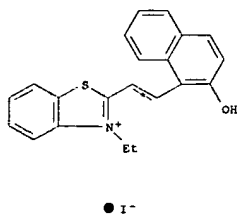
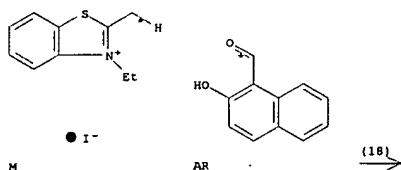


AQ  
YIELD 79%

RX(17) RCT M 3119-93-5, AP 17754-90-4  
PRO AQ 852335-96-7  
CAT 110-89-4 Piperidine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 60 minutes, reflux  
SUBSTAGE(2) reflux -> -18 deg C  
NTE stereoselective

RX(18) OF 21 M + AR ==> AS

L2 ANSWER 4 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



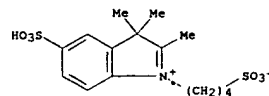
AS  
YIELD 81%

RX(18) RCT M 3119-93-5, AR 708-06-5  
PRO AS 852335-97-8  
CAT 110-89-4 Piperidine  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 60 minutes, reflux  
SUBSTAGE(2) reflux -> -18 deg C  
NTE stereoselective

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 143:22482 CASREACT  
TITLE: Synthesis and application of a water-soluble near-infrared dye for cancer detection using optical imaging  
AUTHOR(S): Pham, Wellington; Medarova, Zdravka; Moore, Anna  
CORPORATE SOURCE: Athinoula A. Martinos Center for Biomedical Imaging, Department of Radiology, Massachusetts General Hospital, Charlestown, MA, 02129, USA  
SOURCE: Bioconjugate Chemistry (2005), 16(3), 735-740  
CODEN: BCCHE5; ISSN: 1043-1802  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB : A novel water-soluble 2-[2-(2-chloro-3-[2-(3,3-dimethyl-5-sulfo-1-(4-sulfo-butyl)-3H-indol-2-yl)]-vinyl)-cyclohex-2-enylidene]-ethylidene]-3,3-dimethyl-1-(4-sulfo-butyl)-1,2,3-dihydro-1H-indole-5-carboxylic acid (dye 2) was developed via an asym. approach. : With an addnl. sulfonate group, the near-IR feature of this dye exhibited a 2-fold increase in quantum yield compared to the previous generation. : The current synthetic strategy provided a single carboxylic group as a handle for conjugation, thus allowing selectivity for bioconjugation. : The stability of this dye was demonstrated by labeling peptides via solid-phase peptide chemical : The in vivo optical imaging showed potential and broad applications of this dye in developing mol.-based beacons for cancer detection.  
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS  
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

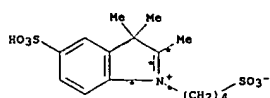
RX(1) OF 17 ...4 A + 2 B + 4 C ==> D + E...



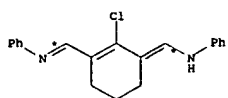
3 A



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

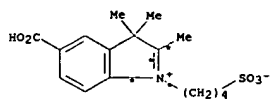


A

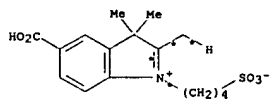


● HCl

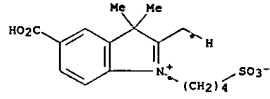
2 B



C



C



C

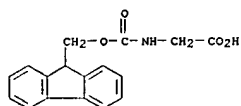
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE (2)

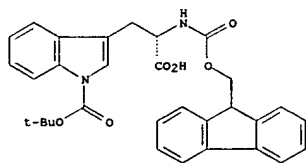
RCT C 852818-04-3  
CON 1 hour, reflux

PRO D 612531-93-8, E 852818-02-1

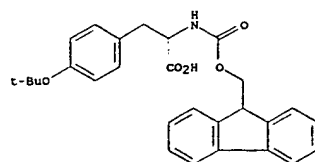
RX(2) OF 17 E ==&gt; R



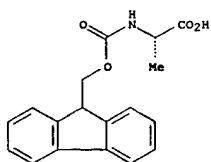
H



I

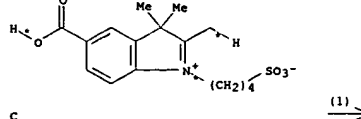


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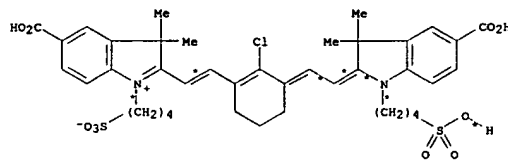
K

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

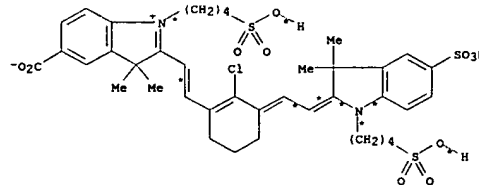


C

(1)



D



E

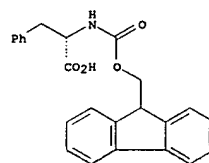
YIELD 9%

RX(1) RCT A 76588-81-3, B 63857-00-1

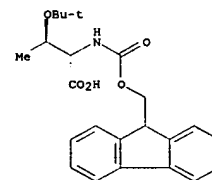
STAGE (1)

RGT F 127-09-3 AcONa  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

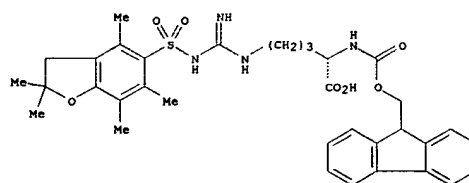
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



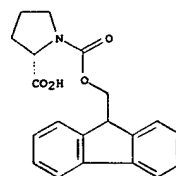
L



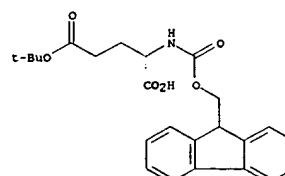
M



N



O

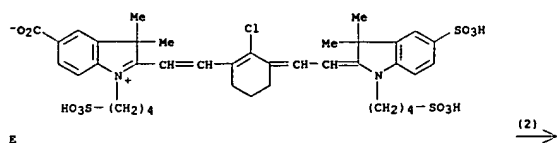


P

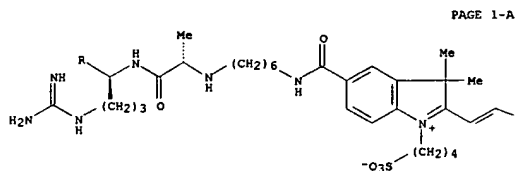
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

H<sub>2</sub>N-(CH<sub>2</sub>)<sub>5</sub>-CO<sub>2</sub>H

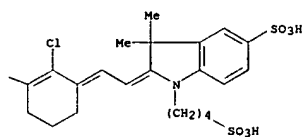
Q



E



PAGE 1-B



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

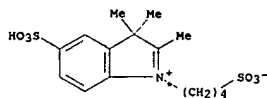
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT H 29022-11-5

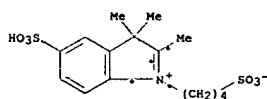
STAGE(1)  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-BenzotriazololSTAGE(2)  
RCT I 143824-78-6  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-BenzotriazololSTAGE(3)  
RCT J 71989-38-3  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-BenzotriazololSTAGE(4)  
RCT K 35661-39-3  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-BenzotriazololSTAGE(5)  
RCT L 35661-40-6  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-BenzotriazololSTAGE(6)  
RCT M 71989-35-0  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-BenzotriazololSTAGE(7)  
RCT N 154445-77-9  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-BenzotriazololSTAGE(8)  
RCT O 71989-31-6  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-BenzotriazololSTAGE(9)  
RCT P 71989-18-9  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-BenzotriazololSTAGE(10)  
RCT Q 60-32-2  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-BenzotriazololSTAGE(11)  
RCT E 852818-02-1  
RGT S 94790-37-1 HBTU, U 110-86-1 Pyridine, T 2592-95-2  
1-Benzotriazolol  
SOL 68-12-2 DMFSTAGE(12)  
RGT V 100-68-5 PhSMe, W 540-63-6 HSCH2CH2SH, X 76-05-1  
F3CCO2H,

Y 100-66-3 PhOMe

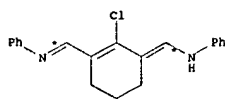
PRO R 852818-03-2

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
NTE solid-supported reaction, Fmoc strategy used, first stage is attachment to Rink amide resinRX(6) OF 17 COMPOSED OF RX(1), RX(2)  
RX(6) 4 A + 2 B + 4 C + H + I + J + K + L + M +  
N + O + P + Q ==> R

3 A

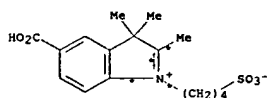


A

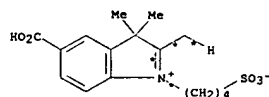


● HCl

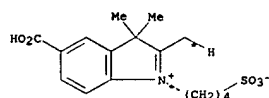
2 B



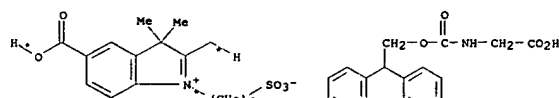
C



C

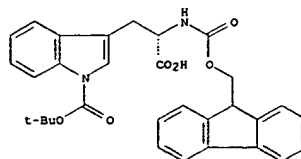


C



C

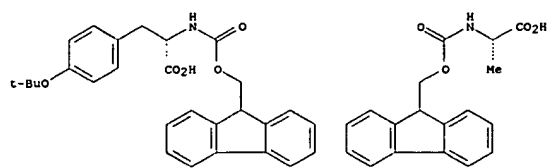
H



I

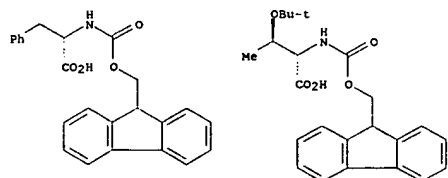
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



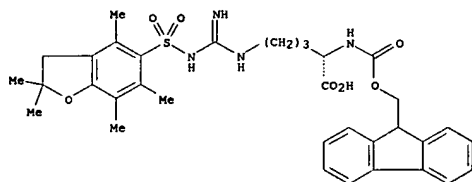
J

K



L

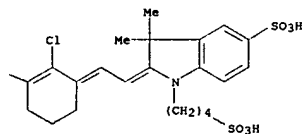
M



N

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 76588-81-3, B 63857-00-1

STAGE(1)

RGT F 127-09-3 ACONA

SOL 64-17-5 EtOH

CON 4 hours, reflux

STAGE(2)

RCT C 852818-04-3

CON 1 hour, reflux

PRO D 612531-93-8, E 852818-02-1

RX(2) RCT H 29022-11-5

STAGE(1)

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(2)

RCT I 143824-78-6

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(3)

RCT J 71989-38-3

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(4)

RCT K 35661-39-3

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(5)

RCT L 35661-40-6

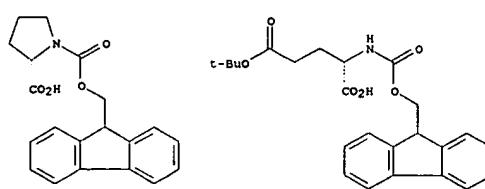
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(6)

RCT M 71989-35-0

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



O

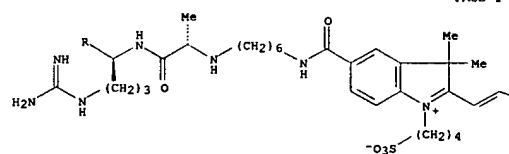
P

H<sub>2</sub>N-(CH<sub>2</sub>)<sub>5</sub>-CO<sub>2</sub>H

Q

2  
STEPS  
→

PAGE 1-A



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(7)

RCT N 154445-77-9

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(8)

RCT O 71989-31-6

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(9)

RCT P 71989-18-9

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(10)

RCT Q 60-32-2

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(11)

RCT E 852818-02-1

RGT S 94790-37-1 HBTU, U 110-86-1 Pyridine, T 2592-95-2

1-Benzotriazolol

SOL 68-12-2 DMF

STAGE(12)

RGT V 100-68-5 PhMe, W 540-63-6 HSCH<sub>2</sub>CH<sub>2</sub>SH, X 76-05-1F3CCO<sub>2</sub>H,

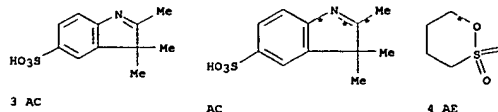
Y 100-66-3 PhOMe

PRO R 852818-03-2

NTE solid-supported reaction, Fmoc strategy used, first stage is attachment to Rink amide resin

RX(8) OF 17 COMPOSED OF RX(4), RX(1)

RX(8) 4 AC + 4 AE + 2 B + 4 C ==&gt; D + E

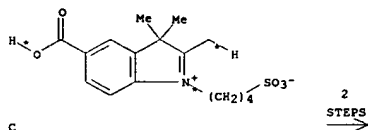
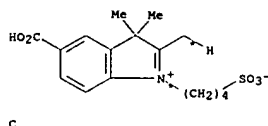
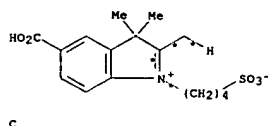
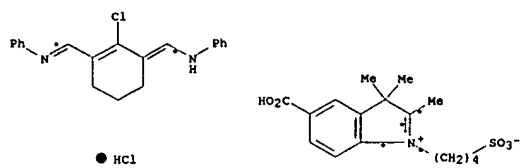


3 AC

AC

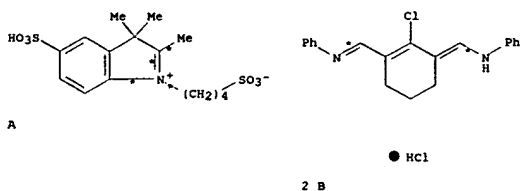
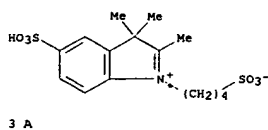
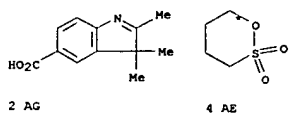
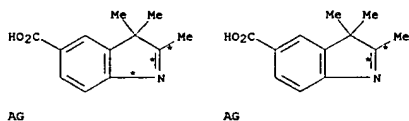
4 AE

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

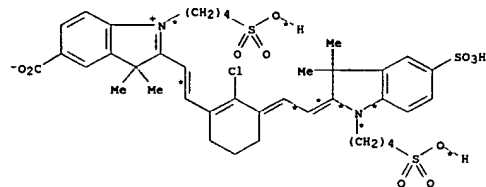
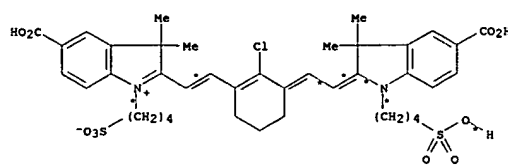


L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(9) OF 17 COMPOSED OF RX(5), RX(1)  
 RX(9) 4 AG + 4 AE + 4 A + 2 B ==> D + E



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



YIELD 9%

RX(4) RCT AC 132557-72-3, AE 1633-83-6  
 PRO A 76588-81-3  
 SOL 95-50-1 o-C6H4Cl2  
 CON 12 hours, 110 deg C

RX(1) RCT A 76588-81-3, B 63857-00-1

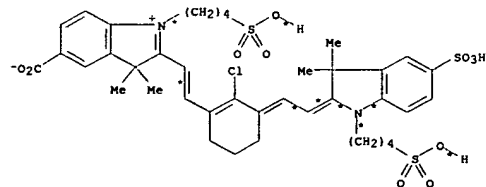
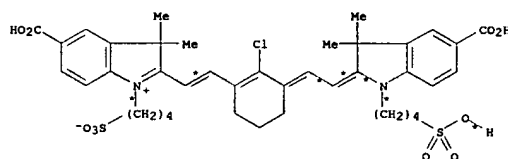
STAGE(1)  
 RGT F 127-09-3 AcONa  
 SOL 64-17-5 EtOH  
 CON 4 hours, reflux

STAGE(2)  
 RCT C 852818-04-3  
 CON 1 hour, reflux

PRO D 612531-93-0, E 852818-02-1

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

2 STEPS



YIELD 9%

RX(5) RCT AG 84100-84-5, AE 1633-83-6  
 PRO C 852818-04-3  
 SOL 95-50-1 o-C6H4Cl2  
 CON 5 hours, reflux

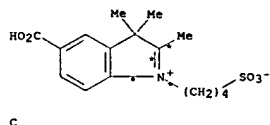
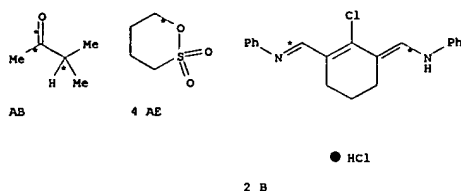
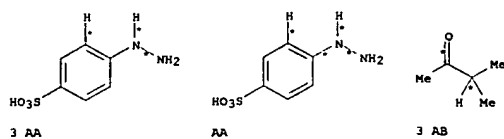
RX(1) RCT A 76588-81-3, B 63857-00-1

STAGE(1)  
 RGT F 127-09-3 AcONa  
 SOL 64-17-5 EtOH  
 CON 4 hours, reflux

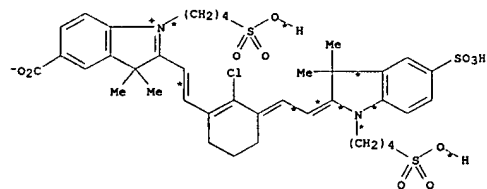
STAGE(2)  
 RCT C 852818-04-3  
 CON 1 hour, reflux

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
PRO D 612531-93-8, E 852818-02-1

RX(10) OF 17 COMPOSED OF RX(3), RX(4), RX(1)  
RX(10) 4 AA + 4 AB + 4 AE + 2 B + 4 C ==> D  
+ E



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



E  
YIELD 9%

RX(3) RCT AA 98-71-5, AB 563-80-4  
RGT F 127-09-3 AcONa  
PRO AC 132557-72-3  
SOL 64-19-7 AcOH  
CON 18 hours, reflux

RX(4) RCT AC 132557-72-3, AE 1633-83-6  
PRO A 76588-81-3  
SOL 95-50-1 o-C6H4Cl2  
CON 12 hours, 110 deg C

RX(1) RCT A 76588-81-3, B 63857-00-1

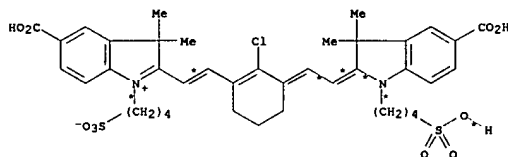
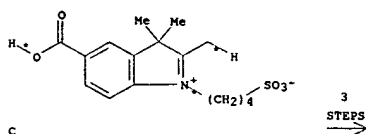
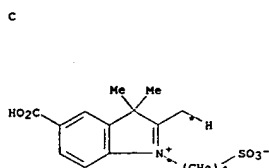
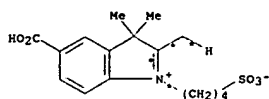
STAGE(1)  
RGT F 127-09-3 AcONa  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

STAGE(2)  
RCT C 852818-04-3  
CON 1 hour, reflux

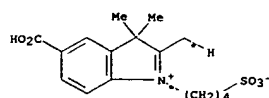
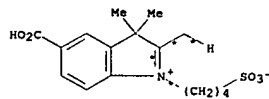
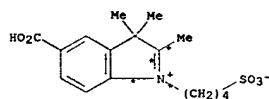
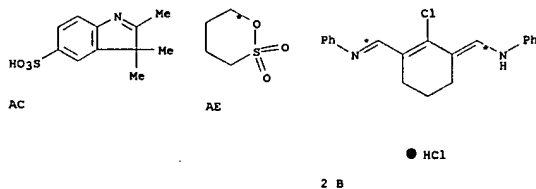
PRO D 612531-93-8, E 852818-02-1

RX(11) OF 17 COMPOSED OF RX(4), RX(1), RX(2)  
RX(11) AC + AE + 2 B + 4 C + H + I + J + K + L +  
M + N + O + P + Q ==> R

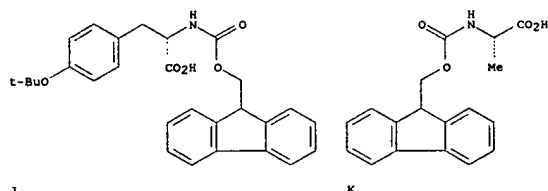
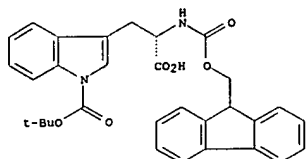
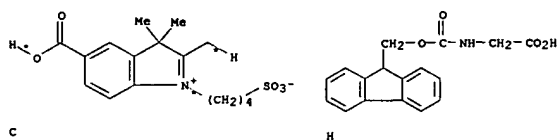
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

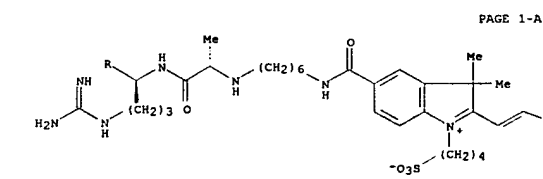


L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

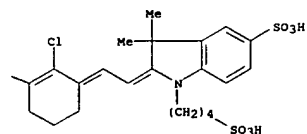
H<sub>2</sub>N<sup>+</sup> (CH<sub>2</sub>)<sub>5</sub><sup>+</sup> CO<sub>2</sub>H

Q

3  
STEPS  
→



PAGE 1-B



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

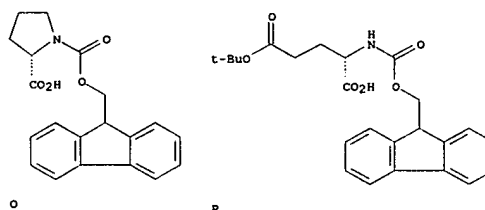
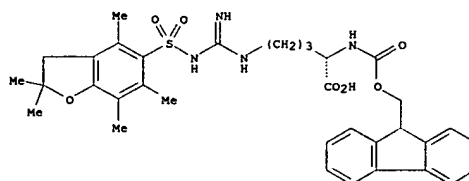
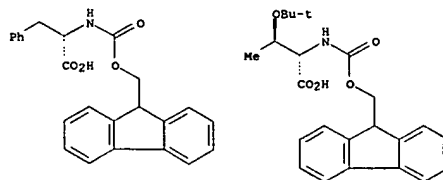
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(4) RCT AC 132557-72-3, AE 1633-83-6  
PRO A 76588-81-3  
SOL 95-50-1 o-C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub>  
CON 12 hours, 110 deg C

RX(1) RCT A 76588-81-3, B 63857-00-1

STAGE(1)  
RGT F 127-09-3 AcONa

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 64-17-5 EtOH  
CON 4 hours, reflux

STAGE(2)  
RCT C 852818-04-3  
CON 1 hour, reflux

PRO D 612531-93-8, E 852818-02-1

RX(2) RCT H 29022-11-5

STAGE(1)  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(2)  
RCT I 143824-78-6  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(3)  
RCT J 71989-38-3  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(4)  
RCT K 35661-39-3  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(5)  
RCT L 35661-40-6  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(6)  
RCT M 71989-35-0  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(7)  
RCT N 154445-77-9  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(8)  
RCT O 71989-31-6  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(9)  
RCT P 71989-18-9  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(10)  
RCT Q 60-32-2  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(11)  
RCT E 852818-02-1  
RGT S 94790-37-1 HBTU, U 110-86-1 Pyridine, T 2592-95-2 1-Benzotriazolol  
SOL 68-12-2 DMF

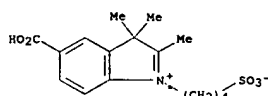
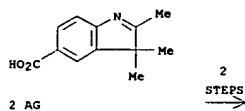
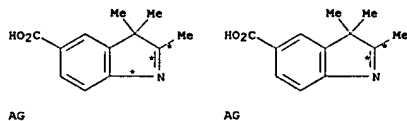
STAGE(12)  
RGT V 100-68-5 PhMe, W 540-63-6 HSCH<sub>2</sub>CH<sub>2</sub>SH, X 76-05-1

F3CCO2H,

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
Y 100-66-3 PhOme

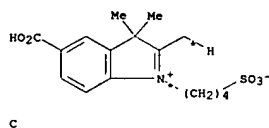
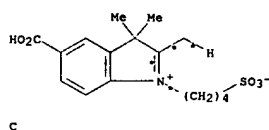
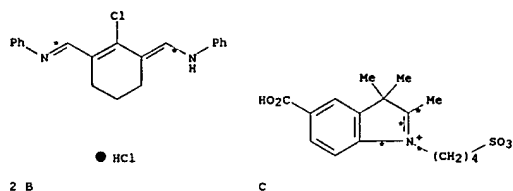
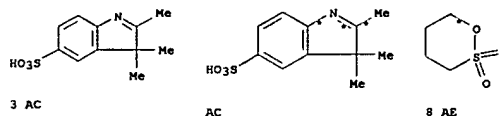
PRO R 852818-03-2  
NTE solid-supported reaction, Fmoc strategy used, first stage is attachment to Rink amide resin

RX(12) OF 17 COMPOSED OF REACTION SEQUENCE RX(5), RX(1)  
AND REACTION SEQUENCE RX(4), RX(1)  
...4 AG + 7 AE ==> C...  
...4 AC + AE + 2 B + 4 C ==> D + E

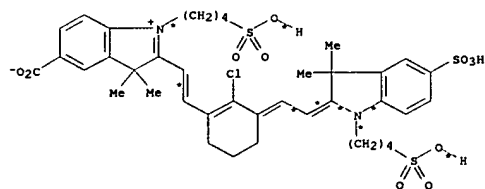
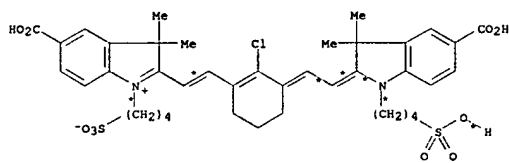
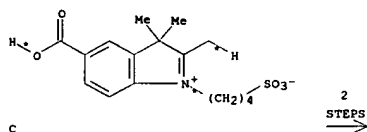


START NEXT REACTION SEQUENCE

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



YIELD 9%

RX(5) RCT AG 84100-84-5, AE 1633-83-6  
PRO C 852818-04-3  
SOL 95-50-1 o-C6H4Cl2  
CON 5 hours, reflux

RX(4) RCT AC 132557-72-3, AE 1633-83-6  
PRO A 76588-81-3  
SOL 95-50-1 o-C6H4Cl2  
CON 12 hours, 110 deg C

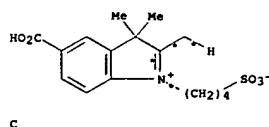
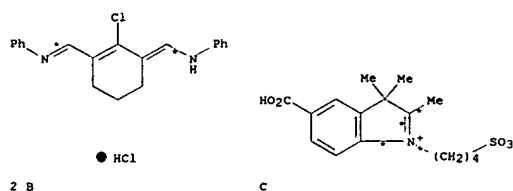
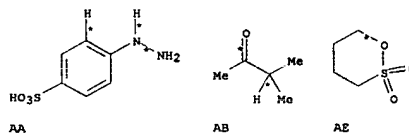
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
RX(1) RCT A 76588-81-3, B 63857-00-1

STAGE(1)  
RGT F 127-09-3 AcONa  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

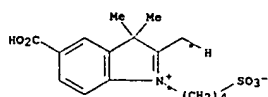
STAGE(2)  
RCT C 852818-04-3  
CON 1 hour, reflux

PRO D 612531-93-8, E 852818-02-1

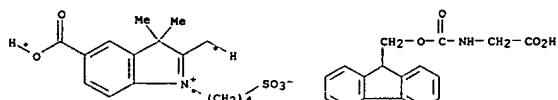
RX(13) OF 17 COMPOSED OF RX(3), RX(4), RX(1), RX(2)  
RX(13) AA + AB + AE + 2 B + 4 C + H + I + J + K +  
L + M + N + O + P + Q ==> R



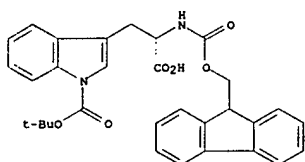
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



C

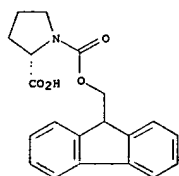


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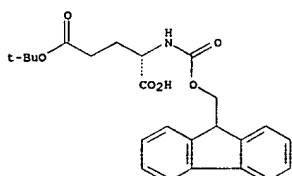


I

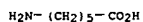
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



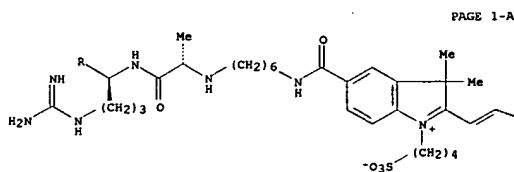
O



P

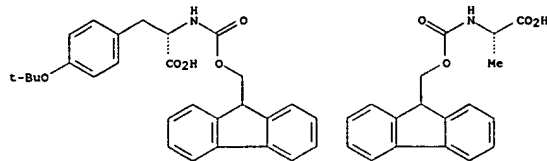


Q

4  
STEPS

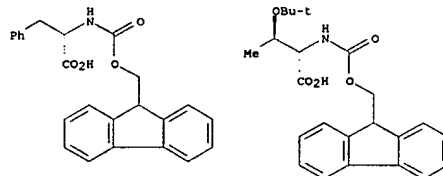
PAGE 1-A

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



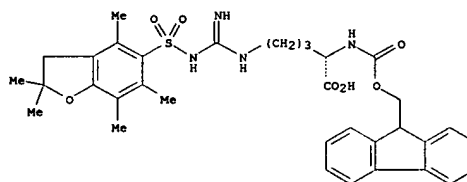
J

K



L

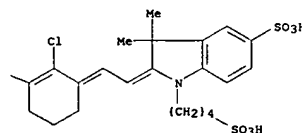
M



N

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(3) RCT AA 98-71-5, AB 563-80-4  
RGT F 127-09-3 AcONa  
PRO AC 132557-72-3  
SOL 64-19-7 AcOH  
CON 18 hours, reflux

RX(4) RCT AC 132557-72-3, AE 1633-83-6  
PRO A 76588-81-3  
SOL 95-50-1 o-C6H4Cl2  
CON 12 hours, 110 deg C

RX(1) RCT A 76588-81-3, B 63857-00-1

STAGE(1)  
RGT F 127-09-3 AcONa  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

STAGE(2)  
RCT C 852818-04-3  
CON 1 hour, reflux

PRO D 612531-93-8, E 852818-02-1

RX(2) RCT H 29022-11-5

STAGE(1)  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(2)  
RCT I 143824-78-6  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(3)  
RCT J 71989-38-3  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(4)



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RCT K 35661-39-3  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(5)

RCT L 35661-40-6  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(6)

RCT M 71989-35-0  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(7)

RCT N 154445-77-9  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(8)

RCT O 71989-31-6  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(9)

RCT P 71989-18-9  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(10)

RCT Q 60-32-2  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(11)

RCT E 852818-02-1  
RGT S 94790-37-1 HBTU, U 110-86-1 Pyridine, T 2592-95-2  
1-Benzotriazolol  
SOL 68-12-2 DMF

STAGE(12)

RGT V 100-68-5 PhMe, W 540-63-6 HSCH<sub>2</sub>CH<sub>2</sub>SH, X 76-05-1

F3CCO<sub>2</sub>H,

Y 100-66-3 PhOMe

PRO R 852818-03-2

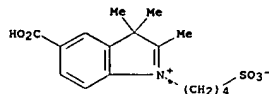
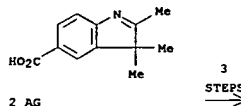
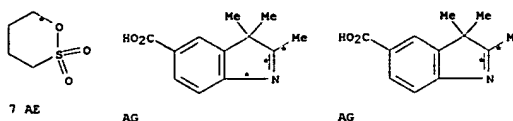
NTE solid-supported reaction, Fmoc strategy used, first stage is  
attachment to Rink amide resin

RX(14) OF 17 COMPOSED OF REACTION SEQUENCE RX(5), RX(1)  
AND REACTION SEQUENCE RX(3), RX(4), RX(1)

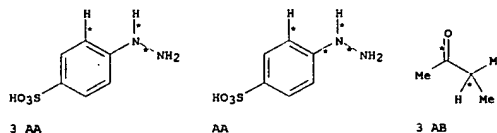
...4 AG + 7 AE ==&gt; C...

...4 AA + 4 AB + AE + 2 B + 4 C ==&gt; D + E

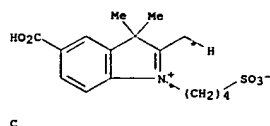
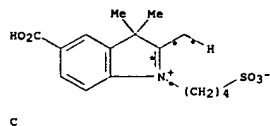
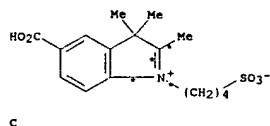
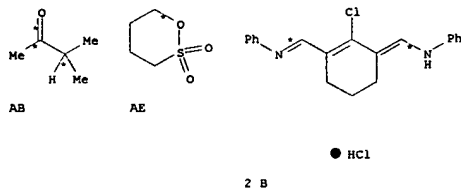
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



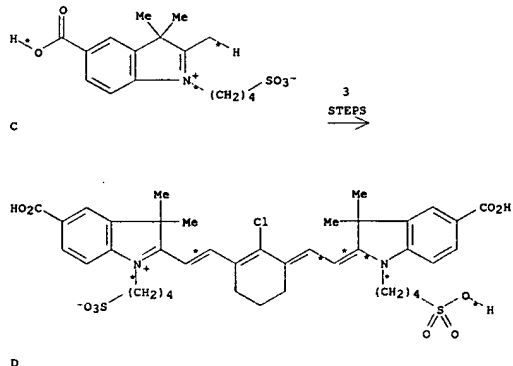
START NEXT REACTION SEQUENCE



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



YIELD 9%

RX(5)      RCT AG 84100-84-5, AE 1633-83-6  
            PRO C 852818-04-3  
            SOL 95-50-1 o-C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub>  
            CON 5 hours, reflux

RX(3)      RCT AA 98-71-5, AB 563-80-4  
            RGT F 127-09-3 AcONa  
            PRO AC 132557-72-3  
            SOL 64-19-7 AcOH

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(4) RCT AC 132557-72-3, AE 1633-83-6  
PRO A 76588-81-3  
SOL 95-50-1 o-C6H4Cl2  
CON 12 hours, 110 deg C

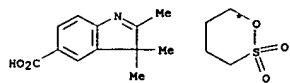
RX(1) RCT A 76588-81-3, B 63857-00-1

STAGE(1)  
RGT F 127-09-3 ACONA  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

STAGE(2)  
RCT C 852818-04-3  
CON 1 hour, reflux

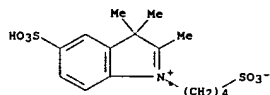
PRO D 612531-93-8, E 852818-02-1

RX(15) OF 17 COMPOSED OF RX(5), RX(1), RX(2)  
RX(15) AG + AE + 4 A + 2 B + H + I + J + K + L +  
M + N + O + P + Q ==> R



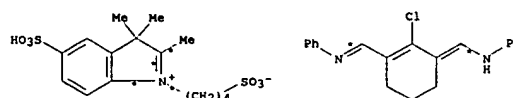
AG

AE



3 A

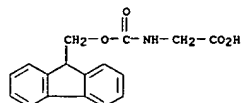
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



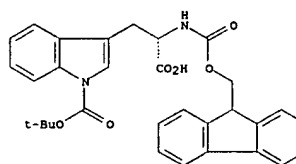
A

● HCl

2 B

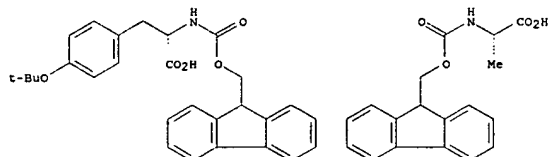


H



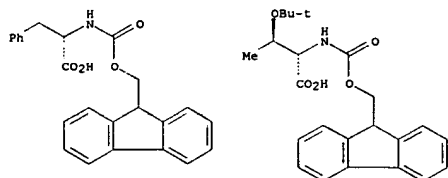
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L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



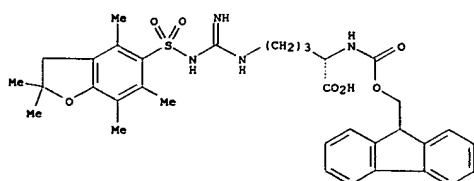
J

K



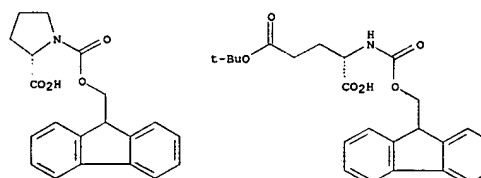
L

M



N

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



O

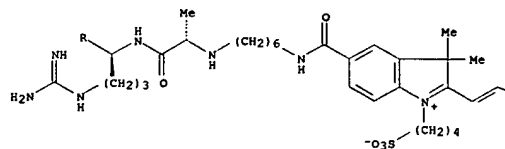
P

H<sub>2</sub>N-(CH<sub>2</sub>)<sub>5</sub>-CO<sub>2</sub>H

Q

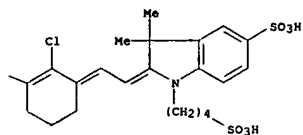
3  
STEPS  
→

PAGE 1-A



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT AG 84100-84-5, AE 1633-83-6  
 PRO C 852818-04-3  
 SOL 95-50-1 o-C6H4Cl2  
 CON 5 hours, reflux

RX(1) RCT A 76588-81-3, B 63857-00-1

STAGE(1)  
 RGT F 127-09-3 AcONa  
 SOL 64-17-5 EtOH  
 CON 4 hours, reflux

STAGE(2)  
 RCT C 852818-04-3  
 CON 1 hour, reflux

PRO D 612531-93-8, E 852818-02-1

RX(2) RCT H 29022-11-5

STAGE(1)  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(2)  
 RCT I 143824-78-6  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(3)  
 RCT J 71989-38-3  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(4)  
 RCT K 35661-39-3  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(5)  
 RCT L 35661-40-6  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(6)  
 RCT M 71989-35-0  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(7)  
 RCT N 154445-77-9  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(8)  
 RCT O 71989-31-6  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(9)  
 RCT P 71989-18-9  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(10)  
 RCT Q 60-32-2  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(11)  
 RCT E 852818-02-1  
 RGT S 94790-37-1 HBTU, U 110-86-1 Pyridine, T 2592-95-2  
 1-Benzotriazolol  
 SOL 68-12-2 DMF

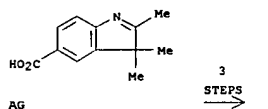
STAGE(12)  
 RGT V 100-68-5 PhSMe, W 540-63-6 HSCH2CH2SH, X 76-05-1  
 F3CCO2H,  
 Y 100-66-3 PhOMe

PRO R 852818-03-2  
 NTE solid-supported reaction, Fmoc strategy used, first stage is  
 attachment to Rink amide resin

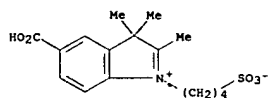
RX(16) OF 17 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(2)  
 AND REACTION SEQUENCE RX(4), RX(1), RX(2)

...AG + AE ==> C...  
 ...AC + AE + 2 B + 4 C + H + I + J + K + L + M +  
 N + O + P + Q ==> R

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

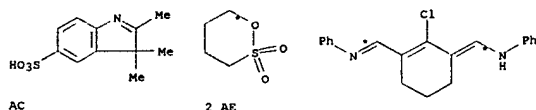


AG

3  
STEPS

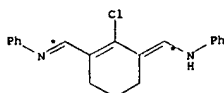
C

START NEXT REACTION SEQUENCE



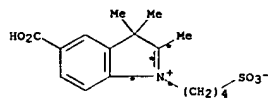
AC

2 AE



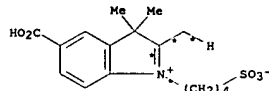
● HCl

2 B

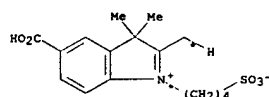


C

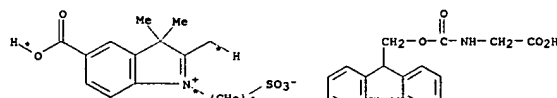
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



C

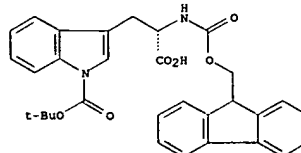


C



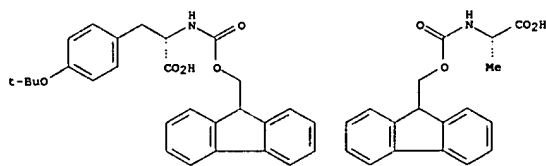
C

H



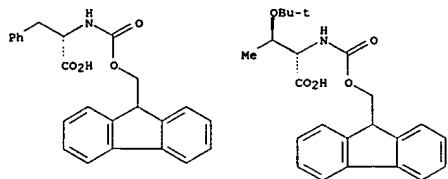
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L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



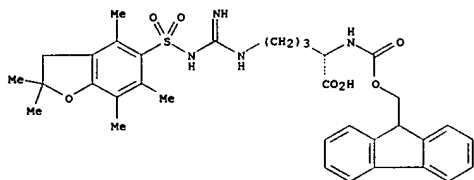
J

K



L

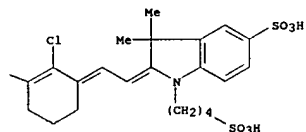
M



N

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-B



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT AG 84100-84-5, AE 1633-83-6  
PRO C 852818-04-3  
SOL 95-50-1 o-C6H4Cl2  
CON 5 hours, reflux

RX(4) RCT AC 132557-72-3, AE 1633-83-6  
PRO A 76588-81-3  
SOL 95-50-1 o-C6H4Cl2  
CON 12 hours, 110 deg C

RX(1) RCT A 76588-81-3, B 63857-00-1

STAGE(1)  
RGT F 127-09-3 AcONa  
SOL 64-17-5 EtOH  
CON 4 hours, reflux

STAGE(2)  
RCT C 852818-04-3  
CON 1 hour, reflux

PRO D 612531-93-8, E 852818-02-1

RX(2) RCT H 29022-11-5

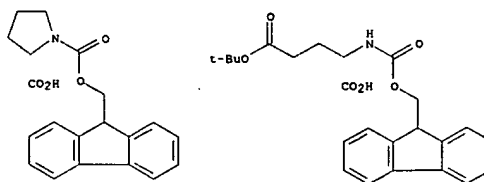
STAGE(1)  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(2)  
RCT I 143824-78-6  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(3)  
RCT J 71989-38-3  
RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(4)  
RCT K 35661-39-3

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



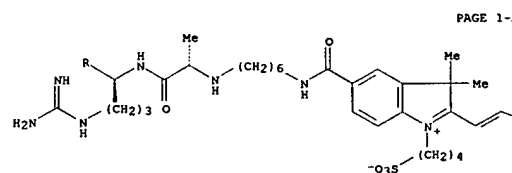
O

P

H<sub>2</sub>N-(CH<sub>2</sub>)<sub>5</sub>-CO<sub>2</sub>H

Q

3  
STEPS



PAGE 1-A

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(5)

RCT L 35661-40-6

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(6)

RCT M 71989-35-0

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(7)

RCT N 154445-77-9

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(8)

RCT O 71989-31-6

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(9)

RCT P 71989-18-9

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(10)

RCT Q 60-32-2

RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(11)

RCT E 852818-02-1

RGT S 94790-37-1 HBTU, U 110-86-1 Pyridine, T 2592-95-2

1-Benzotriazolol

SOL 68-12-2 DMF

STAGE(12)

RGT V 100-68-5 PhMe, W 540-63-6 HSC<sub>2</sub>CH<sub>2</sub>SH, X 76-05-1

Y 100-66-3 PhOMe

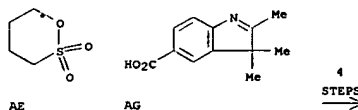
F3CCO<sub>2</sub>H,

PRO R 852818-03-2

NTE solid-supported reaction, Fmoc strategy used, first stage is attachment to Rink amide resin

RX(17) OF 17 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(2)  
AND REACTION SEQUENCE RX(3), RX(4), RX(1), RX(2)

...AG + AE ==> C...  
...AA + AB + AE + 2 B + 4 C + H + I + J + K + L +  
M + N + O + P + Q ==> R

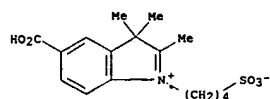


AE

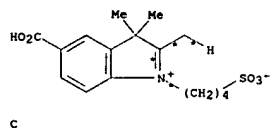
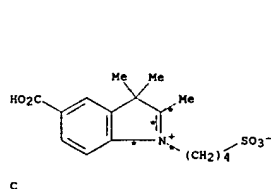
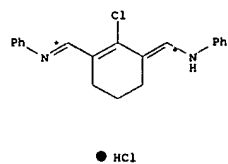
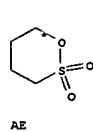
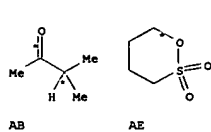
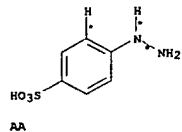
AG

4  
STEPS

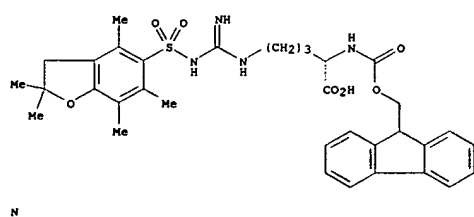
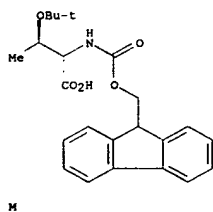
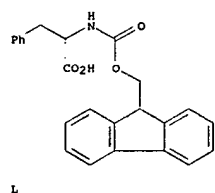
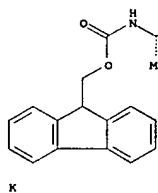
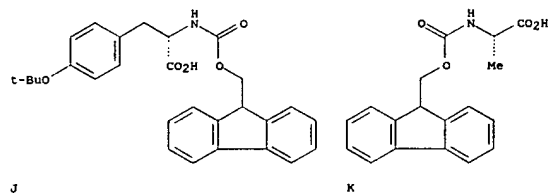
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



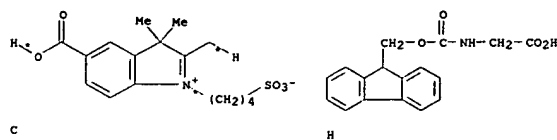
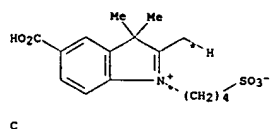
START NEXT REACTION SEQUENCE



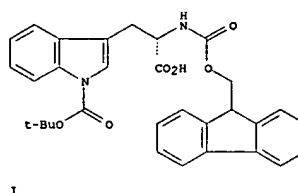
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



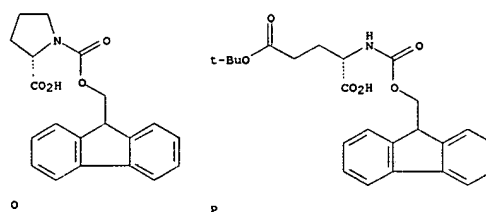
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



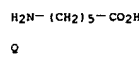
H



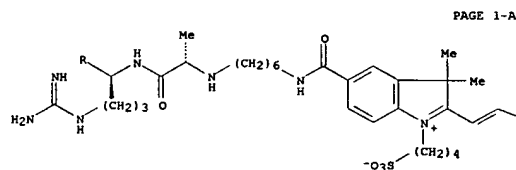
L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



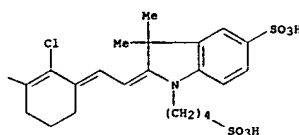
P



4 STEPS



PAGE 1-B



L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*  
 \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT AG 84100-84-5, AE 1633-83-6  
 PRO C 852818-04-3  
 SOL 95-50-1 o-C6H4Cl2  
 CON 5 hours, reflux

RX(3) RCT AA 98-71-5, AB 563-80-4  
 RGT F 127-09-3 AcONa  
 PRO AC 132557-72-3  
 SOL 64-19-7 AcOH  
 CON 18 hours, reflux

RX(4) RCT AC 132557-72-3, AE 1633-83-6  
 PRO A 76588-81-3  
 SOL 95-50-1 o-C6H4Cl2  
 CON 12 hours, 110 deg C

RX(1) RCT A 76588-81-3, B 63857-00-1

STAGE(1)  
 RGT F 127-09-3 AcONa  
 SOL 64-17-5 EtOH  
 CON 4 hours, reflux

STAGE(2)  
 RCT C 852818-04-3  
 CON 1 hour, reflux

PRO D 612531-93-8, E 852818-02-1

RX(2) RCT H 29022-11-5

STAGE(1)  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(2)  
 RCT I 143824-78-6  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(3)  
 RCT J 71989-38-3  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(4)  
 RCT K 35661-39-3  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(5)  
 RCT L 35661-40-6  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(6)

L2 ANSWER 5 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 RCT M 71989-35-0  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(7)  
 RCT N 154445-77-9  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(8)  
 RCT O 71989-31-6  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(9)  
 RCT P 71989-18-9  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(10)  
 RCT Q 60-32-2  
 RGT S 94790-37-1 HBTU, T 2592-95-2 1-Benzotriazolol

STAGE(11)  
 RCT E 852818-02-1  
 RGT S 94790-37-1 HBTU, U 110-86-1 Pyridine, T 2592-95-2  
 1-Benzotriazolol  
 SOL 68-12-2 DMF

STAGE(12)  
 RGT V 100-68-5 PhSMe, W 540-63-6 HSCH2CH2SH, X 76-05-1  
 F3CCO2H, Y 100-66-3 PhOMe

PRO R 852818-03-2  
 NTE solid-supported reaction, Fmoc strategy used, first stage is attachment to Rink amide resin

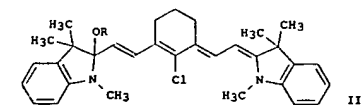
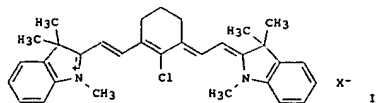
L2 ANSWER 6 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 143:9191 CASREACT  
 TITLE: Nonsolvate-form crystal of polymethine compound and its production process  
 INVENTOR(S): Chichiishi, Keiki; Wada, Sayuri; Fujita, Shigeo  
 PATENT ASSIGNEE(S): Yamamoto Chemicals, Inc., Japan  
 SOURCE: PCT Int. Appl., 34 pp.  
 CODEN: PIKXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005049736	A1	20050602	WO 2004-JP16830	20041112

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RM: BW, CH, GH, KE, LS, MW, MG, NA, SD, SI, SZ, TZ, UG, ZH, ZM, ZW, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

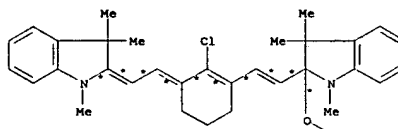
PRIORITY APPL. INFO.: JP 2003-392789 20031121  
 OTHER SOURCE(S): MARPAT 143:9191  
 GI



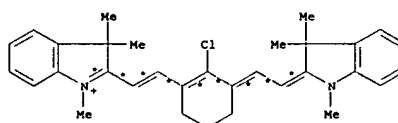
AB The title compound I (X = Cl, Br) useful as near IR absorbers is prepared by reacting a polymethine ether compound II (R = alkyl, alkoxyalkyl, or optionally substituted aryl) with HCl or HBr. Nonsolvate-form crystals of I are satisfactorily stable in solns., have a high gram extinction coefficient

L2 ANSWER 6 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 and excellent storage stability, are easy to handle, and are highly sensitive to common semiconductor lasers.  
 REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(1) OF 2 A ==> B



(1)



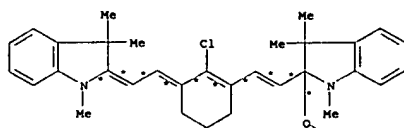
● Cl<sup>-</sup>

B

RX(1) RCT A 819805-22-6  
 RGT C 7647-01-0 HCl  
 PRO B 199444-11-6  
 SOL 67-64-1 Me2CO  
 CON SUBSTAGE(1) 1 hour, 30 deg C  
 SUBSTAGE(2) 30 deg C -> reflux  
 SUBSTAGE(3) 1 hour, reflux

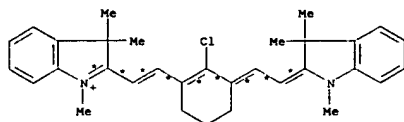
RX(2) OF 2 A ==> E

L2 ANSWER 6 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



A

(2) →

● Br<sup>-</sup>

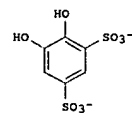
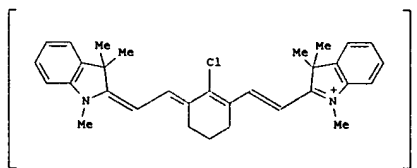
E

RX(2) RCT A 819805-22-6  
 RGT F 10035-10-6 HBr  
 PRO E 212964-63-1  
 SOL 67-64-1 Me2CO  
 CON SUBSTAGE(1) 1 hour, 30 deg C  
 SUBSTAGE(2) 30 deg C -> reflux  
 SUBSTAGE(3) 1 hour, reflux

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 142:483447 CASREACT  
 TITLE: Process for the preparation of infrared absorbing cyanine dyes with polysulfonate anions  
 INVENTOR(S): Tao, Ting; Kottmair, Eduard; Beckley, Scott A.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 15 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

Instant App.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005113546	A1	20050526	US 2003-722257	20031125
EP 1535968	A2	20050601	EP 2004-27416	20041118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR, IS, YU				
JP 2005163039	A2	20050623	JP 2004-340997	20041125
PRIORITY APPLN. INFO.: GI			US 2003-722257	20031125



I

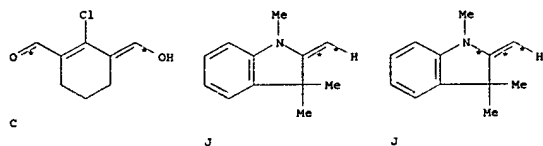
AB A convenient and economical method for preparing IR absorbing cyanine dyes

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 useful in lithog. printing plate precursors is disclosed. The reaction

1s generally carried out by condensation of a heterocyclic base contg. an activated methylene group and an unsatd. bisaldehyde or its equiv. in a solvent or solvent mixt. at about 20-150°. All the reactions necessary for prodn. of the IR absorbing cyanine dye may be carried out

1n one reaction vessel without isolating any intermediate products. Thus, 2-chloro-1-formyl-3-hydroxymethylencyclohexene was reacted with 1,3,3-trimethyl-2-methyleneindoline (Fisher's base) to give a dark-green soln. which was then added to a soln. contg. disodium 4,5-dihydroxy-1,3-benzenedisulfonate to give a ppt. of an IR absorbing cyanine dye (I).

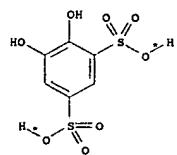
RX(3) OF 14 ...C + 2 J + K ==> L



C

J

J

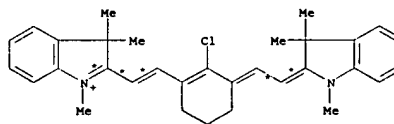


● 2 Na

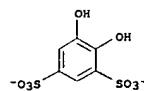
K

(3) →

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L: CM 1



L: CM 2

RX(3) RCT C 61010-04-6, J 118-12-7

STAGE(1)  
 CAT 7647-01-0 HCl, 127-09-3 AcONa  
 SOL 7732-18-5 Water, 64-17-5 EtOH  
 CON SUBSTAGE(1) 6 hours, 70 deg C  
 SUBSTAGE(2) 70 deg C -> room temperature

STAGE(2)  
 RGT E 7732-18-5 Water  
 CON room temperature

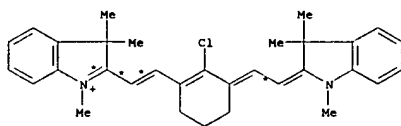
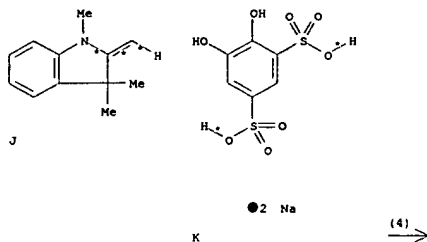
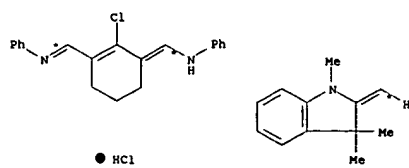
STAGE(3)  
 RCT K 149-45-1  
 SOL 7732-18-5 Water, 64-17-5 EtOH  
 CON room temperature

PRO L 518052-03-4

RX(4) OF 14 ...G + 2 J + K ==> L

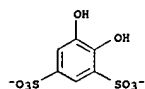
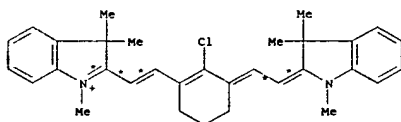
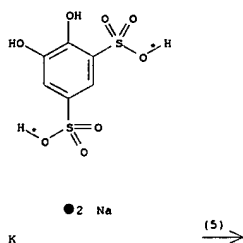
L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



RX(5) RCT C 61010-04-6, J 118-12-7

STAGE(1)

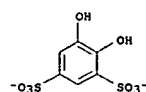
RGT H 7647-01-0 HCl  
 SOL 7732-18-5 Water, 71-43-2 Benzene, 71-23-8 ProH  
 CON 3 hours, 100 deg C

STAGE(2)

RCT K 149-45-1  
 SOL 7732-18-5 Water, 64-17-5 EtOH  
 CON room temperature

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



L: CH 2

RX(4) RCT G 63857-00-1, J 118-12-7

STAGE(1)

SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 4 hours, 70 deg C  
 SUBSTAGE(2) 70 deg C → room temperature

STAGE(2)

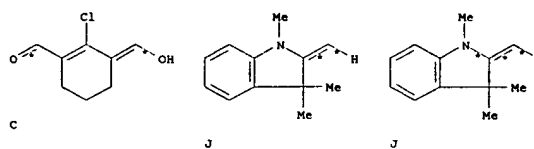
RGT E 7732-18-5 Water  
 CON room temperature

STAGE(3)

RCT K 149-45-1  
 SOL 7732-18-5 Water, 64-17-5 EtOH  
 CON room temperature

PRO L 518052-03-4

RX(5) OF 14 C + 2 J + K ==&gt; L

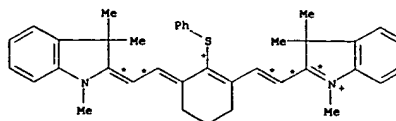
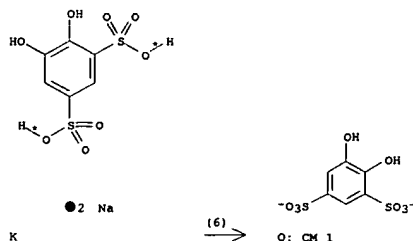
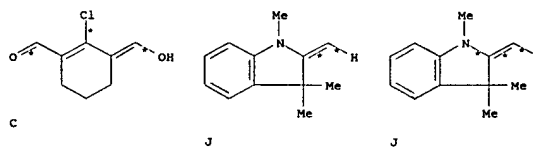


L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

PRO L 518052-03-4

(Continued)

RX(6) OF 14 ...C + 2 J + P + K ==&gt; Q





L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(6) RCT C 61010-04-6, J 118-12-7

## STAGE(1)

CAT 7647-01-0 HCl, 127-09-3 AcONa  
 SOL 7732-18-5 Water, 64-17-5 EtOH  
 CON SUBSTAGE(1) 7 hours, 70 deg C  
 SUBSTAGE(2) 70 deg C -> room temperature

## STAGE(2)

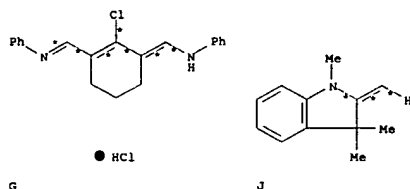
RCT P 108-98-5  
 RGT R 1310-73-2 NaOH  
 SOL 64-17-5 EtOH  
 CON 15 hours, room temperature

## STAGE(3)

RCT K 149-45-1  
 SOL 7732-18-5 Water, 64-17-5 EtOH  
 CON room temperature

PRO Q 491576-85-3

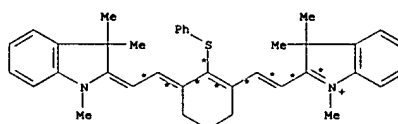
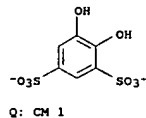
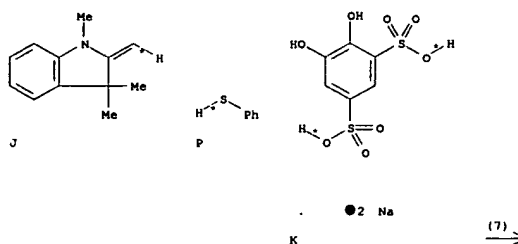
RX(7) OF 14 ...G + 2 J + P + K ==&gt; Q



G

J

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(7) RCT G 63857-00-1, J 118-12-7

## STAGE(1)

SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 4 hours, 70 deg C  
 SUBSTAGE(2) 70 deg C -> room temperature

## STAGE(2)

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RCT P 108-98-5  
 RGT R 1310-73-2 NaOH  
 SOL 64-17-5 EtOH  
 CON 15 hours, room temperature

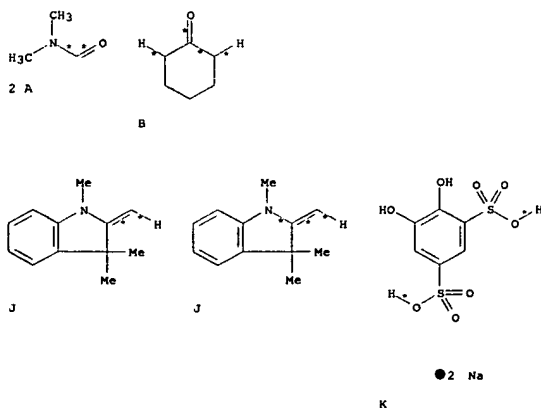
## STAGE(3)

RGT H 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON 42 deg C

## STAGE(4)

RCT K 149-45-1  
 SOL 7732-18-5 Water

PRO Q 491576-85-3

RX(9) OF 14 COMPOSED OF RX(1), RX(3)  
RX(9) 2 A + B + 2 J + K ==> L

2 A

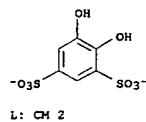
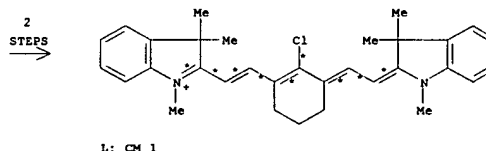
B

J

J

K

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(1) RCT A 68-12-2

## STAGE(1)

RGT D 10025-87-3 POCl3  
 CON SUBSTAGE(1) cooled  
 SUBSTAGE(2) 1 hour, 10 - 15 deg C  
 SUBSTAGE(3) 30 minutes, 15 deg C -> room temperature

## STAGE(2)

RCT B 108-94-1  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) 40 - 50 deg C  
 SUBSTAGE(2) 3 hours, 55 deg C

## STAGE(3)

RGT E 7732-18-5 Water  
 CON SUBSTAGE(1) cooled  
 SUBSTAGE(2) 15 hours

PRO C 61010-04-6

RX(3) RCT C 61010-04-6, J 118-12-7

## STAGE(1)

CAT 7647-01-0 HCl, 127-09-3 AcONa  
 SOL 7732-18-5 Water, 64-17-5 EtOH  
 CON SUBSTAGE(1) 6 hours, 70 deg C  
 SUBSTAGE(2) 70 deg C -> room temperature

## STAGE(2)

RGT E 7732-18-5 Water  
 CON room temperature

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(3)

RCT K 149-45-1

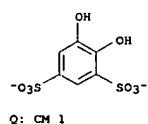
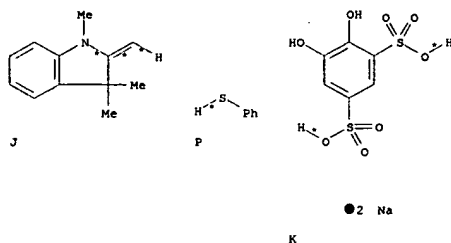
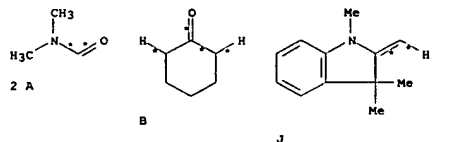
SOL 7732-18-5 Water, 64-17-5 EtOH

CON room temperature

PRO L 510052-03-4

RX(10) OF 14 COMPOSED OF RX(1), RX(6)

RX(10) 2 A + B + 2 J + P + K ==&gt; Q

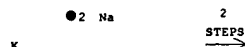
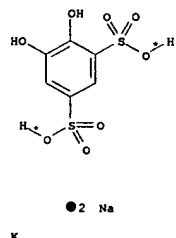
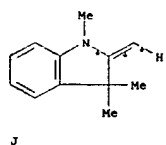
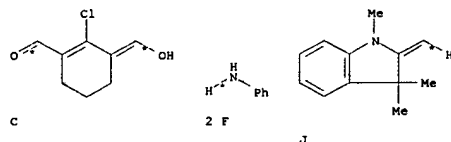


L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

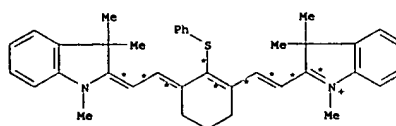
PRO Q 491576-85-3

RX(11) OF 14 COMPOSED OF RX(2), RX(4)

RX(11) C + 2 F + 2 J + K ==&gt; L



L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



Q: CH 2

RX(1) RCT A 68-12-2

STAGE(1)

RGT D 10025-87-3 POCl3

CON SUBSTAGE(1) cooled

SUBSTAGE(2) 1 hour, 10 - 15 deg C

SUBSTAGE(3) 30 minutes, 15 deg C -&gt; room temperature

STAGE(2)

RCT B 108-94-1

SOL 68-12-2 DMF

CON SUBSTAGE(1) 40 - 50 deg C

SUBSTAGE(2) 3 hours, 55 deg C

STAGE(3)

RGT E 7732-18-5 Water

CON SUBSTAGE(1) cooled

SUBSTAGE(2) 15 hours

PRO C 61010-04-6

RX(6) RCT C 61010-04-6, J 110-12-7

STAGE(1)

CAT 7647-01-0 HCl, 127-09-3 AcONa

SOL 7732-18-5 Water, 64-17-5 EtOH

CON SUBSTAGE(1) 7 hours, 70 deg C

SUBSTAGE(2) 70 deg C -&gt; room temperature

STAGE(2)

RCT P 108-98-5

RGT R 1310-73-2 NaOH

SOL 64-17-5 EtOH

CON 15 hours, room temperature

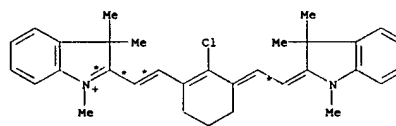
STAGE(3)

RCT K 149-45-1

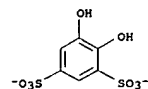
SOL 7732-18-5 Water, 64-17-5 EtOH

CON room temperature

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L: CH 1



L: CH 2

RX(2) RCT C 61010-04-6, F 62-53-3

STAGE(1)

RGT H 7647-01-0 HCl

SOL 7732-18-5 Water, 64-17-5 EtOH, 68-12-2 DMF

CON 20 minutes, 15 - 20 deg C

STAGE(2)

RGT E 7732-18-5 Water

CON 20 minutes

PRO G 63857-00-1

NTE safety, mixing of HCl with DMF is highly exothermic

RX(4) RCT G 63857-00-1, J 110-12-7

STAGE(1)

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 4 hours, 70 deg C

SUBSTAGE(2) 70 deg C -&gt; room temperature

STAGE(2)

RGT E 7732-18-5 Water

CON room temperature

STAGE(3)

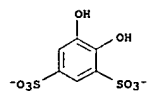
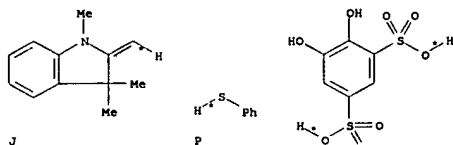
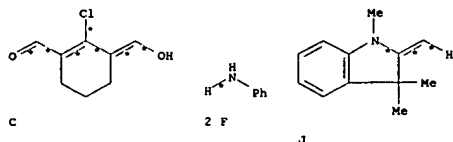
RCT K 149-45-1

SOL 7732-18-5 Water, 64-17-5 EtOH

CON room temperature

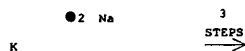
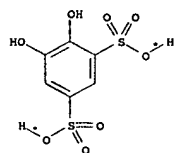
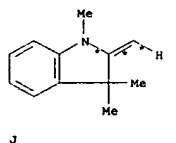
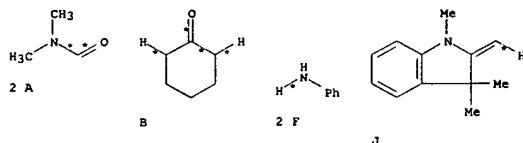
PRO L 510052-03-4

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 RX(12) OF 14 COMPOSED OF RX(2), RX(7)  
 RX(12) C + 2 F + 2 J + P + K ==> Q

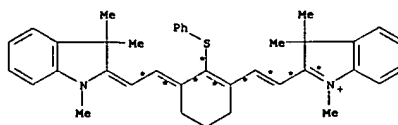


Q: CH 1

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 RX(13) 2 A + B + 2 F + 2 J + K ==> L



L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



Q: CH 2

RX(2) RCT C 61010-04-6, F 62-53-3

STAGE(1)  
 RGT H 7647-01-0 HCl  
 SOL 7732-18-5 Water, 64-17-5 EtOH, 68-12-2 DMF  
 CON 20 minutes, 15 - 20 deg C

STAGE(2)  
 RGT E 7732-18-5 Water  
 CON 20 minutes

PRO G 63857-00-1  
 NTE safety, mixing of HCl with DMF is highly exothermic

RX(7) RCT G 63857-00-1, J 118-12-7

STAGE(1)  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) 4 hours, 70 deg C  
 SUBSTAGE(2) 70 deg C -> room temperature

STAGE(2)  
 RCT P 108-98-5  
 RGT R 1310-73-2 NaOH  
 SOL 64-17-5 EtOH  
 CON 15 hours, room temperature

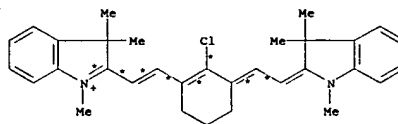
STAGE(3)  
 RGT H 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON 42 deg C

STAGE(4)  
 RCT K 149-45-1  
 SOL 7732-18-5 Water

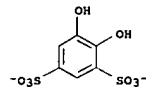
PRO Q 491576-85-3

RX(13) OF 14 COMPOSED OF RX(1), RX(2), RX(4)

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L: CH 1



L: CH 2

RX(1) RCT A 68-12-2

STAGE(1)  
 RGT D 10025-87-3 POCl3  
 CON SUBSTAGE(1) cooled  
 SUBSTAGE(2) 1 hour, 10 - 15 deg C  
 SUBSTAGE(3) 30 minutes, 15 deg C -> room temperature

STAGE(2)  
 RCT B 108-94-1  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) 40 - 50 deg C  
 SUBSTAGE(2) 3 hours, 55 deg C

STAGE(3)  
 RGT E 7732-18-5 Water  
 CON SUBSTAGE(1) cooled  
 SUBSTAGE(2) 15 hours

PRO C 61010-04-6

RX(2) RCT C 61010-04-6, F 62-53-3

STAGE(1)  
 RGT H 7647-01-0 HCl  
 SOL 7732-18-5 Water, 64-17-5 EtOH, 68-12-2 DMF  
 CON 20 minutes, 15 - 20 deg C

STAGE(2)  
 RGT E 7732-18-5 Water  
 CON 20 minutes

PRO G 63857-00-1

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
MTE safety, mixing of HCl with DMF is highly exothermic

RX(4) RCT G 63857-00-1, J 110-12-7

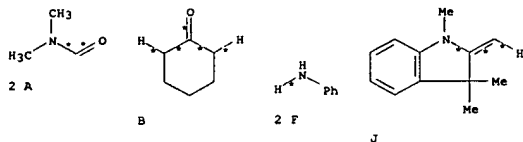
STAGE(1)  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 70 deg C  
SUBSTAGE(2) 70 deg C -> room temperature

STAGE(2)  
RGT E 7732-18-5 Water  
CON room temperature

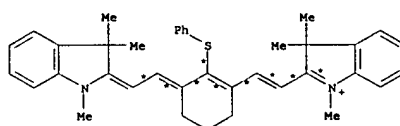
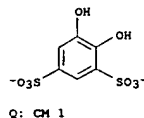
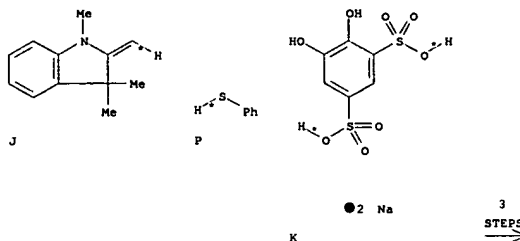
STAGE(3)  
RCT K 149-45-1  
SOL 7732-18-5 Water, 64-17-5 EtOH  
CON room temperature

PRO L 518052-03-4

RX(14) OF 14 COMPOSED OF RX(1), RX(2), RX(7)  
RX(14) 2 A + B + 2 F + 2 J + P + K ==> Q



L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



Q: CH 2

RX(1) RCT A 68-12-2

STAGE(1)  
RGT D 10025-87-3 POCl3  
CON SUBSTAGE(1) cooled  
SUBSTAGE(2) 1 hour, 10 - 15 deg C  
SUBSTAGE(3) 30 minutes, 15 deg C -> room temperature

L2 ANSWER 7 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(2)  
RCT B 108-94-1  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) 40 - 50 deg C  
SUBSTAGE(2) 3 hours, 55 deg C

STAGE(3)  
RGT E 7732-18-5 Water  
CON SUBSTAGE(1) cooled  
SUBSTAGE(2) 15 hours

PRO C 61010-04-6

RX(2) RCT C 61010-04-6, F 62-53-3

STAGE(1)  
RGT H 7647-01-0 HCl  
SOL 7732-18-5 Water, 64-17-5 EtOH, 68-12-2 DMF  
CON 20 minutes, 15 - 20 deg C

STAGE(2)  
RGT E 7732-18-5 Water  
CON 20 minutes

PRO G 63857-00-1  
MTE safety, mixing of HCl with DMF is highly exothermic

RX(7) RCT G 63857-00-1, J 110-12-7

STAGE(1)  
SOL 64-17-5 EtOH  
CON SUBSTAGE(1) 4 hours, 70 deg C  
SUBSTAGE(2) 70 deg C -> room temperature

STAGE(2)  
RCT P 108-98-5  
RGT R 1310-73-2 NaOH  
SOL 64-17-5 EtOH  
CON 15 hours, room temperature

STAGE(3)  
RGT H 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 42 deg C

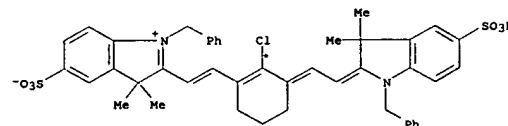
STAGE(4)  
RCT K 149-45-1  
SOL 7732-18-5 Water

PRO Q 491576-85-3

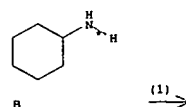
L2 ANSWER 8 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:431579 CASREACT  
TITLE: Heptamethine cyanine dyes with a large Stokes shift and strong fluorescence: A paradigm for excited-state intramolecular charge transfer  
AUTHOR(S): Peng, Xiaojun; Song, Fengling; Lu, Erhu; Wang, Yanan; Zhou, Wei; Fan, Jiangli; Gao, Yunling  
CORPORATE SOURCE: State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian, 116012, Peop. Rep. China  
SOURCE: Journal of the American Chemical Society (2005), 127(12), 4170-4171  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB New heptamethine cyanine dyes with an alkylamino group at the central position were found to exhibit a large Stokes shift (>140 nm) and strong fluorescence. They were suggested to be a new paradigm for excited-state intramolecular charge transfer (ICT). The configuration change of the bridgehead amine accompanying the ICT was investigated in different viscosity and pH media.  
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

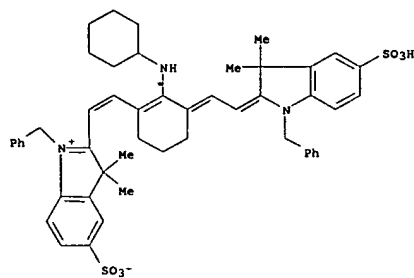
RX(1) OF 2 A + B ==> C



A



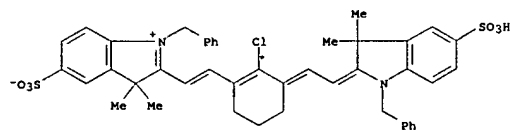
L2 ANSWER 8 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



C

RX(1) RCT A 850612-21-4, B 108-91-8  
 STAGE(1)  
 SOL 68-12-2 DMF  
 CON 2 hours, 68 - 70 deg C  
 STAGE(2)  
 SOL 60-29-7 Et2O  
 PRO C 850612-19-0

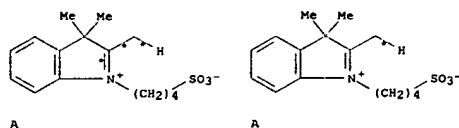
RX(2) OF 2 A + F ==&gt; G



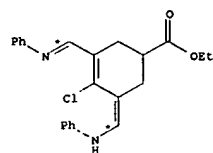
A

L2 ANSWER 9 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 142:431577 CASREACT  
 TITLE: Synthesis of a functionalized cyanine dye for  
 covalent labeling of biomolecules with a pH-sensitive  
 chromophore  
 AUTHOR(S): Strekowski, Lucjan; Mason, Christian C.; Lee, Hyeran;  
 Patonay, Gabor  
 CORPORATE SOURCE: Department of Chemistry, Georgia State University,  
 Atlanta, GA, 30303, USA  
 SOURCE: Heterocyclic Communications (2004), 10(6), 381-382  
 CODEN: HCOMEX; ISSN: 0793-0283  
 PUBLISHER: Freund Publishing House Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A cyanine dye was obtained which has a hydroxy group on the central meso  
 position of the heptamethine chain for pH sensitivity (pKa of about 4.5  
 with lambda max of 715 nm and 535 nm in aqueous MeOH under acidic and  
 neutral/basic conditions, resp.) and is can be functionalized with a  
 [(succinimido)oxy]carbonyl group (N-hydroxysuccinimide ester) for  
 selective reaction with primary amines.  
 REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(1) OF 6 2 A + B ==&gt; C...



A

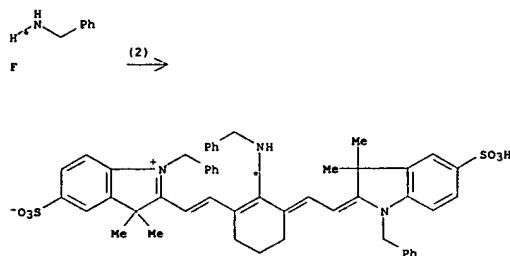


● HCl

B

(1) →

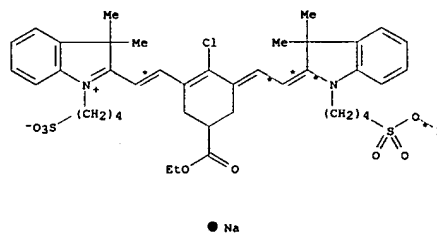
L2 ANSWER 8 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



G

RX(2) RCT A 850612-21-4, F 100-46-9  
 STAGE(1)  
 SOL 68-12-2 DMF  
 CON 1 hour, 80 deg C  
 STAGE(2)  
 SOL 60-29-7 Et2O  
 PRO G 850612-27-0

L2 ANSWER 9 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

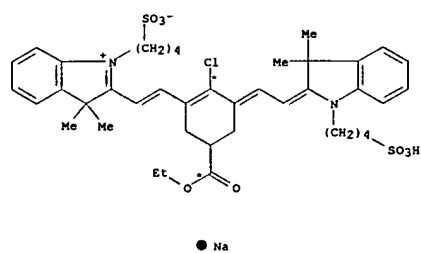


● Na

C  
YIELD 59%

RX(1) RCT A 54136-26-4, B 710337-83-0  
 RGT D 127-09-3 AcONa  
 PRO C 850694-05-2  
 SOL 64-17-5 EtOH

RX(2) OF 6 ...C ==&gt; F...

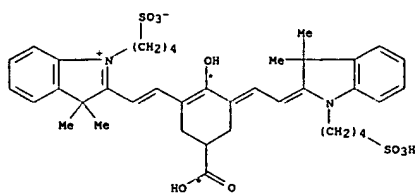


● Na

C

(2) →

L2 ANSWER 9 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

F  
YIELD 67%

RX(2) RCT C 850694-05-2

STAGE(1)  
RGT G 124-41-4 NaOMe  
SOL 67-56-1 MeOH  
CON 12 hours, reflux

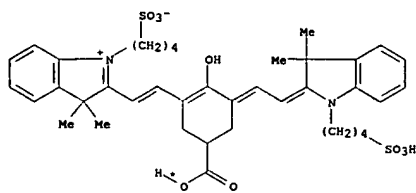
STAGE(2)  
RGT H 7681-82-5 NaI  
SOL 68-12-2 DMF  
CON 12 hours, 80 deg C

STAGE(3)  
RGT I 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO F 850694-06-3

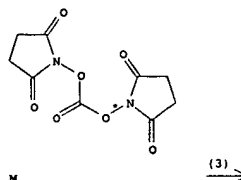
RX(3) OF 6 ...F + M ==&gt; N

L2 ANSWER 9 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

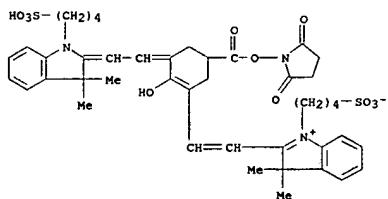
F



M

(3) →

L2 ANSWER 9 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

N  
YIELD 90%

RX(3) RCT F 850694-06-3, M 74124-79-1

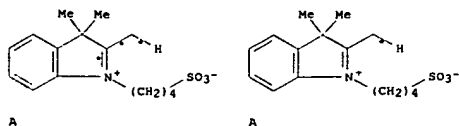
STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, room temperature

STAGE(2)  
SOL 60-29-7 Et2O  
CON room temperature

PRO N 850694-07-4

RX(4) OF 6 COMPOSED OF RX(1), RX(2)

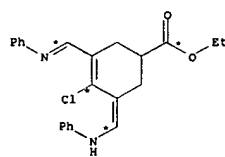
RX(4) 2 A + B ==> F



A

A

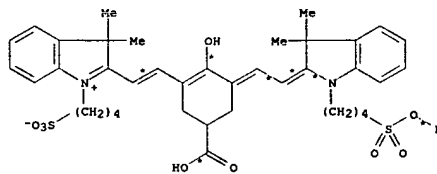
L2 ANSWER 9 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● HCl

2  
STEPS  
→

B



● Na

F  
YIELD 67%

RX(1) RCT A 54136-26-4, B 710337-83-0  
RGT D 127-09-3 AcONa  
PRO C 850694-05-2  
SOL 64-17-5 EtOH

RX(2) RCT C 850694-05-2

STAGE(1)  
RGT G 124-41-4 NaOMe  
SOL 67-56-1 MeOH  
CON 12 hours, reflux

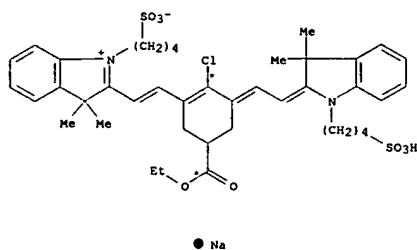
STAGE(2)  
RGT H 7681-82-5 NaI  
SOL 68-12-2 DMF

L2 ANSWER 9 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
CON 12 hours, 80 deg C

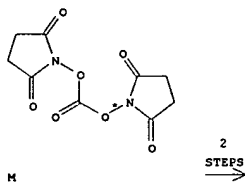
STAGE(3)  
RGT I 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO F 850694-06-3

RX(5) OF 6 COMPOSED OF RX(2), RX(3)  
RX(5) C + M ==> N



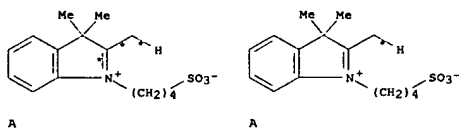
C



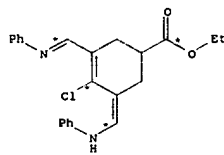
M

L2 ANSWER 9 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

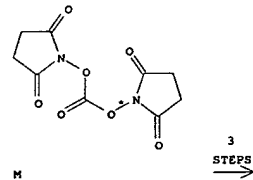
RX(6) OF 6 COMPOSED OF RX(1), RX(2), RX(3)  
RX(6) 2 A + B + M ==> N



A

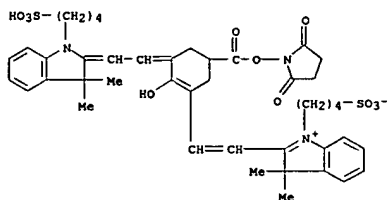


B



M

L2 ANSWER 9 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

N  
YIELD 90%

RX(2) RCT C 850694-05-2

STAGE(1)  
RGT G 124-41-4 NaOMe  
SOL 67-56-1 MeOH  
CON 12 hours, reflux

STAGE(2)  
RGT H 7681-82-5 NaI  
SOL 68-12-2 DMF  
CON 12 hours, 80 deg C

STAGE(3)  
RGT I 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO F 850694-06-3

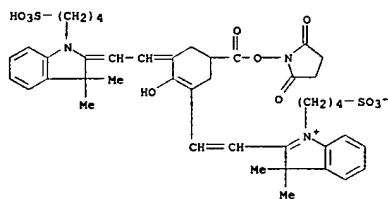
RX(3) RCT F 850694-06-3, M 74124-79-1

STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, room temperature

STAGE(2)  
SOL 60-29-7 Et2O  
CON room temperature

PRO N 850694-07-4

L2 ANSWER 9 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

N  
YIELD 90%

RX(1) RCT A 54136-26-4, B 710337-83-0  
RGT D 127-09-3 AcONa  
PRO C 850694-05-2  
SOL 64-17-5 EtOH

RX(2) RCT C 850694-05-2

STAGE(1)  
RGT G 124-41-4 NaOMe  
SOL 67-56-1 MeOH  
CON 12 hours, reflux

STAGE(2)  
RGT H 7681-82-5 NaI  
SOL 68-12-2 DMF  
CON 12 hours, 80 deg C

STAGE(3)  
RGT I 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO F 850694-06-3

RX(3) RCT F 850694-06-3, M 74124-79-1

STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, room temperature

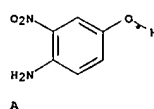
STAGE(2)  
SOL 60-29-7 Et2O  
CON room temperature

PRO N 850694-07-4

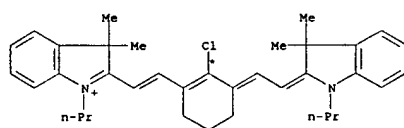
L2 ANSWER 9 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 142:426312 CASREACT  
 TITLE: Highly Sensitive Near-Infrared Fluorescent Probes for Nitric Oxide and Their Application to Isolated Organs  
 AUTHOR(S): Sasaki, Elta; Kojima, Hirotatsu; Nishimatsu, Hiroaki; Urano, Yasuteru; Kikuchi, Kazuya; Hirata, Yasunobu; Nagano, Tetsuo  
 CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, and Faculty of Medicine, The University of Tokyo, Bunkyo, Tokyo, 113-0033, Japan  
 SOURCE: Journal of the American Chemical Society (2005), 127(11), 3684-3685  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Novel near-IR (NIR) fluorescent probes for nitric oxide (NO) have been designed, synthesized, and evaluated. Their NIR fluorescence was increased in an NO concentration-dependent manner under physiologic conditions, and their reaction efficiency with NO was at least 53 times higher than that of a widely used NO probe, DAF-2. They were confirmed to function in isolated intact rat kidneys. Because NIR light can penetrate deeply into tissues, these probes may have potential for in vivo NO imaging.  
 REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

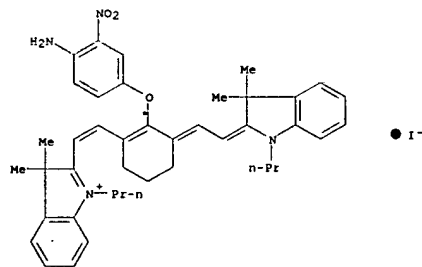
RX(1) OF 18 A + B ==&gt; C...



L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● I<sup>-</sup>

(1) →



YIELD 72%

RX(1) RCT A 610-81-1

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 10 minutes, room temperature

STAGE(2)

RCT B 207399-07-3

SOL 68-12-2 DMF

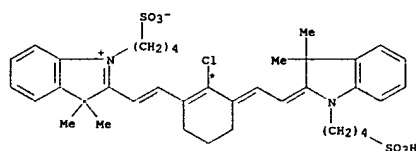
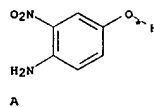
CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 4 hours, room temperature

PRO C 849745-18-2

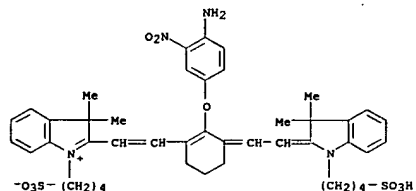
L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(2) OF 18 A + F ==&gt; G...



● Na

(2) →



● Na

YIELD 85%



L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(2) RCT A 610-81-1

## STAGE(1)

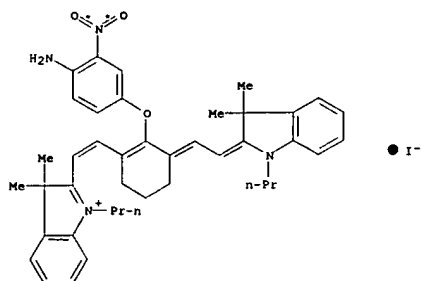
RGT D 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 10 minutes, room temperature

## STAGE(2)

RCT F 115970-66-6  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 4 hours, room temperature

PRO G 849745-23-9

RX(3) OF 18 ...C ==&gt; H...



(3) →

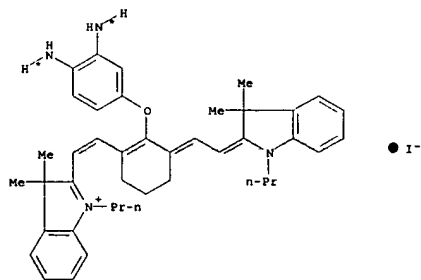
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(3) RCT C 849745-18-2

## STAGE(1)

RGT I 10025-69-1 SnCl<sub>2</sub>·2H<sub>2</sub>O, J 7647-01-0 HCl  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON overnight, room temperature

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



(5) →

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5)

## STAGE(1)

RGT P 10102-43-9 Nitrogen oxide (NO)  
SOL 67-56-1 MeOH  
CON room temperature

## STAGE(2)

RCT H 849745-28-4  
SOL 67-56-1 MeOH  
CON room temperature

PRO O 849745-41-1

RX(6) OF 18 ...M ==&gt; Q

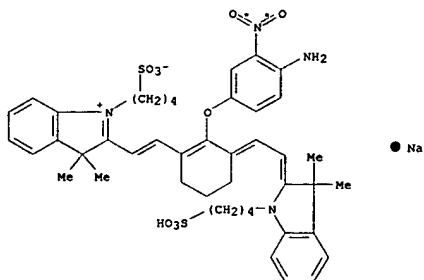
L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

## STAGE(2)

RGT K 1310-73-2 NaOH  
SOL 7732-18-5 Water  
CON room temperature, neutralized

PRO H 849745-28-4

RX(4) OF 18 ...O ==&gt; N...



(4) →

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(4) RCT G 849745-23-9

## STAGE(1)

RGT I 10025-69-1 SnCl<sub>2</sub>·2H<sub>2</sub>O, J 7647-01-0 HCl  
SOL 7732-18-5 Water, 67-56-1 MeOH  
CON overnight, room temperature

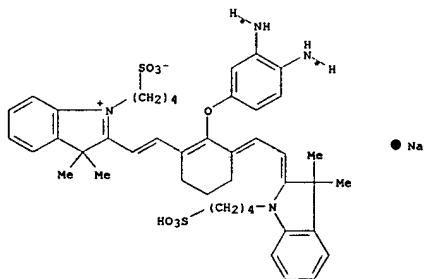
## STAGE(2)

RGT K 1310-73-2 NaOH  
SOL 7732-18-5 Water  
CON room temperature, neutralized

PRO N 849745-34-2

RX(5) OF 18 ...H ==&gt; O

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



(6) →

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(6)

## STAGE(1)

RGT P 10102-43-9 Nitrogen oxide (NO)  
SOL 67-56-1 MeOH  
CON room temperature

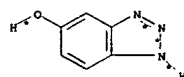
## STAGE(2)

RCT N 849745-34-2  
SOL 67-56-1 MeOH  
CON room temperature

PRO Q 849745-46-6

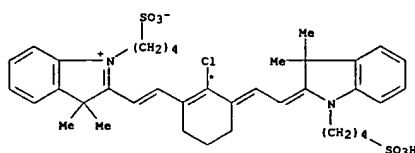
NTE alternate preparation also described

RX(9) OF 18 ...U + F ==&gt; Q



U

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

(9) →

F

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(9) RCT U 54013-40-0

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 10 minutes, room temperature

STAGE(2)

RCT F 115970-66-6

SOL 68-12-2 DMF

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 6 hours, room temperature

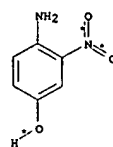
PRO Q 849745-46-6

NTE alternate preparation also described

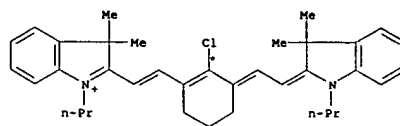
RX(10) OF 18 COMPOSED OF RX(1), RX(3)

RX(10) A + B ==&gt; H

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



A



● I-

2  
STEPS  
→

B

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 610-81-1

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 10 minutes, room temperature

STAGE(2)

RCT B 207399-07-3

SOL 68-12-2 DMF

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 4 hours, room temperature

PRO C 849745-18-2

RX(3) RCT C 849745-18-2

STAGE(1)

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RGT I 10025-69-1 SnCl2.2H2O, J 7647-01-0 HCl

SOL 7732-18-5 Water, 67-56-1 MeOH

CON overnight, room temperature

STAGE(2)

RGT K 1310-73-2 NaOH

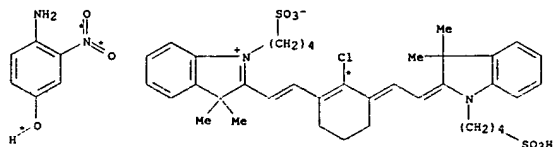
SOL 7732-18-5 Water

CON room temperature, neutralized

PRO H 849745-28-4

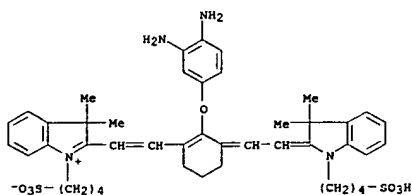
RX(11) OF 18 COMPOSED OF RX(2), RX(4)

RX(11) A + F ==&gt; H



● Na

F

2  
STEPS  
→

● Na

N  
YIELD 20%

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(2) RCT A 610-81-1

STAGE(1)

RGT D 7646-69-7 NaH

SOL 68-12-2 DMF

CON 10 minutes, room temperature

STAGE(2)

RCT F 115970-66-6

SOL 68-12-2 DMF

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 4 hours, room temperature

PRO G 849745-23-9

RX(4) RCT G 849745-23-9

STAGE(1)

RGT I 10025-69-1 SnCl2.2H2O, J 7647-01-0 HCl

SOL 7732-18-5 Water, 67-56-1 MeOH

CON overnight, room temperature

STAGE(2)

RGT K 1310-73-2 NaOH

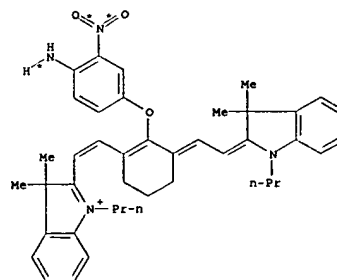
SOL 7732-18-5 Water

CON room temperature, neutralized

PRO N 849745-34-2

RX(12) OF 18 COMPOSED OF RX(3), RX(5)

RX(12) C ==&gt; O



● I-

2  
STEPS  
→

C

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(3) RCT C 849745-10-2

## STAGE(1)

RGT I 10025-69-1 SnCl<sub>2</sub>·2H<sub>2</sub>O, J 7647-01-0 HCl  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON overnight, room temperature

## STAGE(2)

RGT K 1310-73-2 NaOH  
 SOL 7732-18-5 Water  
 CON room temperature, neutralized

PRO H 849745-20-4

RX(5)

## STAGE(1)

RGT P 10102-43-9 Nitrogen oxide (NO)  
 SOL 67-56-1 MeOH  
 CON room temperature

## STAGE(2)

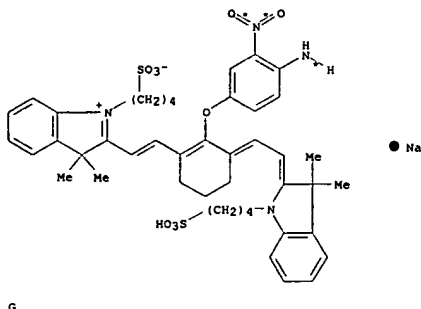
RGT H 849745-20-4  
 SOL 67-56-1 MeOH  
 CON room temperature

PRO O 849745-41-1

RX(13) OF 18 COMPOSED OF RX(4), RX(6)

RX(13) G ==&gt; Q

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(4) RCT G 849745-23-9

## STAGE(1)

RGT I 10025-69-1 SnCl<sub>2</sub>·2H<sub>2</sub>O, J 7647-01-0 HCl  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON overnight, room temperature

## STAGE(2)

RGT K 1310-73-2 NaOH  
 SOL 7732-18-5 Water  
 CON room temperature, neutralized

PRO N 849745-34-2

RX(6)

## STAGE(1)

RGT P 10102-43-9 Nitrogen oxide (NO)  
 SOL 67-56-1 MeOH  
 CON room temperature

## STAGE(2)

RGT N 849745-34-2  
 SOL 67-56-1 MeOH  
 CON room temperature

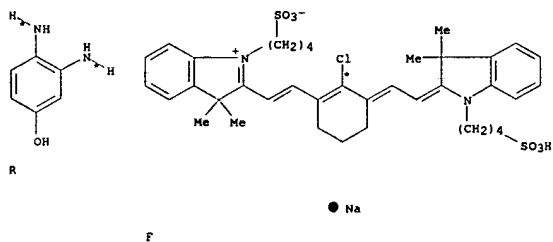
L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO Q 849745-46-6

NTE alternate preparation also described

RX(15) OF 18 COMPOSED OF RX(8), RX(9)

RX(15) R + F ==&gt; Q

2  
STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(8) RCT R 615-72-5

## STAGE(1)

RGT J 7647-01-0 HCl, V 7632-00-0 NaNO<sub>2</sub>  
 SOL 7732-18-5 Water  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 1.5 hours, room temperature

## STAGE(2)

RGT K 1310-73-2 NaOH  
 SOL 7732-18-5 Water  
 CON room temperature, neutralized

PRO U 54013-40-0

RX(9) RCT U 54013-40-0

## STAGE(1)

RGT D 7646-69-7 NaH  
 SOL 68-12-2 DMF  
 CON 10 minutes, room temperature

## STAGE(2)

RGT F 115970-66-6

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 68-12-2 DMF

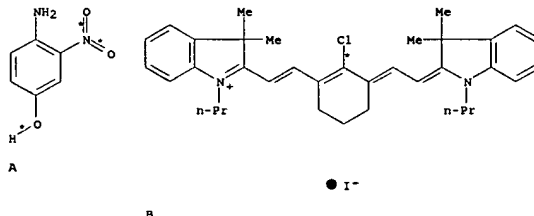
CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 6 hours, room temperature

PRO Q 849745-46-6

NTE alternate preparation also described

RX(16) OF 18 COMPOSED OF RX(1), RX(3), RX(5)

RX(16) A + B ==&gt; O

3  
STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 610-81-1

## STAGE(1)

RGT D 7646-69-7 NaH  
 SOL 68-12-2 DMF  
 CON 10 minutes, room temperature

## STAGE(2)

RGT B 207399-07-3  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 4 hours, room temperature

PRO C 849745-10-2

RX(3) RCT C 849745-10-2

## STAGE(1)

RGT I 10025-69-1 SnCl<sub>2</sub>·2H<sub>2</sub>O, J 7647-01-0 HCl  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON overnight, room temperature

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(2)  
 RGT K 1310-73-2 NaOH  
 SOL 7732-18-5 Water  
 CON room temperature, neutralized

PRO H 849745-28-4

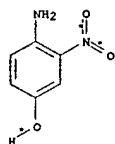
RX(5)

STAGE(1)  
 RGT P 10102-43-9 Nitrogen oxide (NO)  
 SOL 67-56-1 MeOH  
 CON room temperature

STAGE(2)  
 RCT H 849745-28-4  
 SOL 67-56-1 MeOH  
 CON room temperature

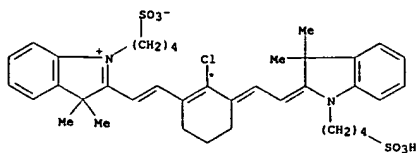
PRO O 849745-41-1

RX(17) OF 18 COMPOSED OF RX(2), RX(4), RX(6)  
 RX(17) A + F ==> Q



A

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

3  
STEPS  
→

F

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT A 610-81-1

STAGE(1)  
 RGT D 7646-69-7 NaH  
 SOL 68-12-2 DMF  
 CON 10 minutes, room temperature

STAGE(2)  
 RCT F 115970-66-6  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 4 hours, room temperature

PRO G 849745-23-9

RX(4) RCT G 849745-23-9

STAGE(1)  
 RGT I 10025-69-1 SnCl2.2H2O, J 7647-01-0 HCl  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON overnight, room temperature

STAGE(2)  
 RGT K 1310-73-2 NaOH  
 SOL 7732-18-5 Water  
 CON room temperature, neutralized

PRO N 849745-34-2

RX(6)

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

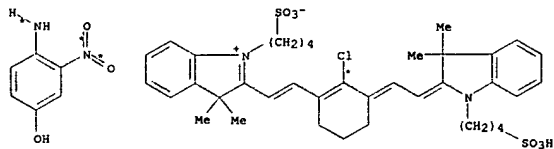
STAGE(1)  
 RGT P 10102-43-9 Nitrogen oxide (NO)  
 SOL 67-56-1 MeOH  
 CON room temperature

STAGE(2)  
 RCT N 849745-34-2  
 SOL 67-56-1 MeOH  
 CON room temperature

PRO Q 849745-46-6

NTE alternate preparation also described

RX(18) OF 18 COMPOSED OF RX(7), RX(8), RX(9)  
 RX(18) A + F ==> Q



A

● Na

F

3

STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(7) RCT A 610-81-1  
 RGT S 1333-74-0 H2  
 PRO R 615-72-5  
 CAT 7440-05-3 Pd  
 SOL 67-56-1 MeOH  
 CON 3 hours, room temperature

RX(8) RCT R 615-72-5

STAGE(1)  
 RGT J 7647-01-0 HCl, V 7632-00-0 NaN2O  
 SOL 7732-18-5 Water  
 CON SUBSTAGE(1) 0 deg C

L2 ANSWER 10 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SUBSTAGE(2) 1.5 hours, room temperature

STAGE(2)  
 RGT K 1310-73-2 NaOH  
 SOL 7732-18-5 Water  
 CON room temperature, neutralized

PRO U 54013-40-0

RX(9) RCT U 54013-40-0

STAGE(1)  
 RGT D 7646-69-7 NaH  
 SOL 68-12-2 DMF  
 CON 10 minutes, room temperature

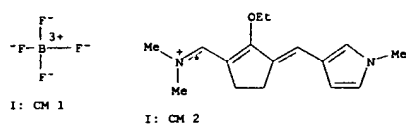
STAGE(2)  
 RCT F 115970-66-6  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 6 hours, room temperature

PRO Q 849745-46-6

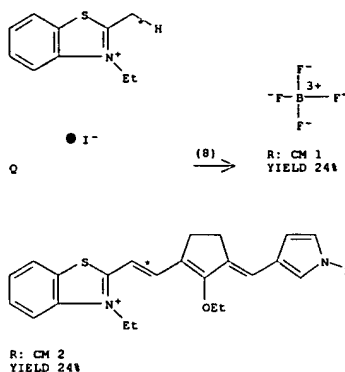
NTE alternate preparation also described

L2 ANSWER 11 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 141:297358 CASREACT  
 TITLE: Protonation and alkylation of cross-conjugated ketones  
 containing a terminal N-methylpyrrole ring  
 AUTHOR(S): Kraanaya, Zh. A.; Smirnova, Yu. V.  
 CORPORATE SOURCE: N. D. Zelinsky Institute of Organic Chemistry,  
 Russian Academy of Sciences, Moscow, 117913, Russia  
 SOURCE: Chemistry of Heterocyclic Compounds (New York, NY,  
 United States)(Translation of Khimiya  
 Geterotsiklicheskikh Soedinenii) (2003), 39(10),  
 1307-1313  
 CODEN: CHCCAL; ISSN: 0009-3122  
 PUBLISHER: Kluwer Academic/Consultants Bureau  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The protonation and alkylation of cross-conjugated ketones containing a  
 terminal N-methylpyrrole ring takes place at the oxygen atom.  
 Protonation is accompanied by a strong bathochromic shift of the absorption maximum  
 in the electronic spectrum, while alkylation leads to ethoxypolymethine  
 salts. The possibility of using these salts for the synthesis of  
 ethoxycyanine dyes was studied.  
 REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(8) OF 9 ...I + Q ==> R

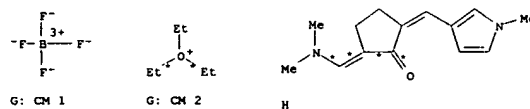


L2 ANSWER 11 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

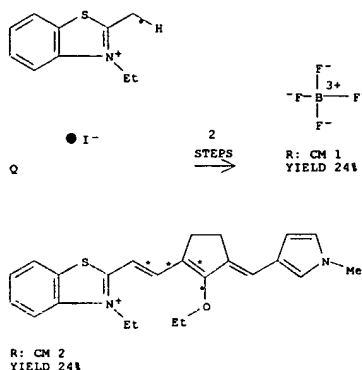


RX(8) RCT I 763123-02-0, Q 3119-93-5  
 RGT S 121-44-8 Et3N  
 PRO R 763123-12-2  
 SOL 108-24-7 Ac2O  
 CON SUBSTAGE(1) 5 minutes, 20 deg C  
 SUBSTAGE(2) 40 minutes, 0 deg C

RX(9) OF 9 COMPOSED OF RX(3), RX(8)  
 RX(9) G + H + Q ==> R



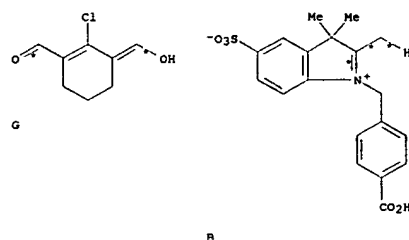
L2 ANSWER 11 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



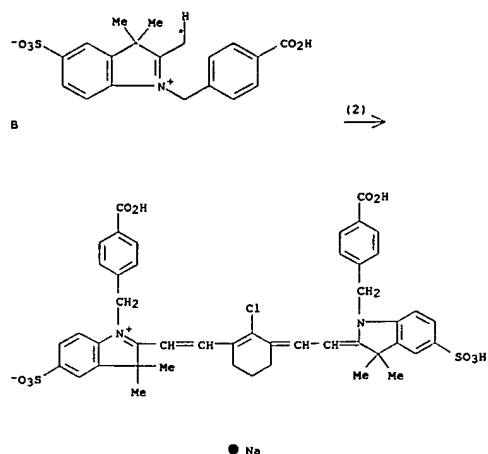
RX(3) RCT G 368-39-8, H 182188-05-2  
 PRO I 763123-02-0  
 SOL 75-09-2 CH2Cl2  
 CON SUBSTAGE(1) -10 deg C  
 SUBSTAGE(2) 1 hour, -19 ~ -15 deg C  
 NTE stereoselective, E:Z 1:3  
 RX(8) RCT I 763123-02-0, Q 3119-93-5  
 RGT S 121-44-8 Et3N  
 PRO R 763123-12-2  
 SOL 108-24-7 Ac2O  
 CON SUBSTAGE(1) 5 minutes, 20 deg C  
 SUBSTAGE(2) 40 minutes, 0 deg C

L2 ANSWER 12 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 141:244919 CASREACT  
 TITLE: New near-infrared indocyanines and their spectral  
 properties in SiO2 sol-gel  
 AUTHOR(S): Wang, Liqiu; Peng, Xiaojun; Song, Fengling; Lu, Erhu;  
 Cui, Jingnan; Gao, Xinglin; Lu, Rogwen  
 CORPORATE SOURCE: State Key Laboratory of Fine Chemicals, Dalian  
 University of Technology, Dalian, 116012, Peop. Rep.  
 China  
 SOURCE: Dyes and Pigments (2004), 61(2), 103-107  
 CODEN: DYPIOX; ISSN: 0143-7208  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB To improve the stability and spectral properties, new heptamethine  
 3H-indocyanine dyes were synthesized and tested in solvents and SiO2  
 sol-gel. The results show that the dyes containing cyclohexenylene  
 bridge and N-(4-carboxybenzyl) groups have better photostability and longer  
 absorption wavelengths than those containing a linear heptamethine bridge  
 and/or N-(5-carboxypentyl) groups. The absorption maxima are in inverse  
 proportion to the polarity of the solvents in which they are determined  
 When dyes doped in SiO2 sol-gel, the absorption maxima are between those in  
 methanol and in DMF.  
 REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(2) OF 8 ...G + 2 B ==> H



L2 ANSWER 12 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

H  
YIELD 29%

RX(2) RCT G 61010-04-6, B 749259-68-5

## STAGE(1)

RGT I 127-09-3 AcONa  
SOL 108-24-7 Ac2O  
CON 6 hours, room temperature

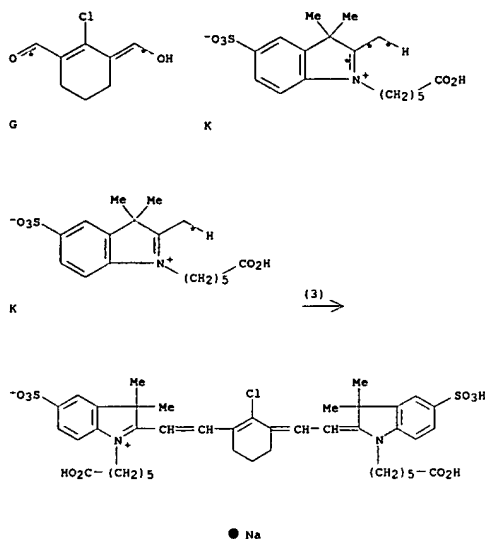
## STAGE(2)

RGT J 141-78-6 AcOEt  
CON room temperature

PRO H 749259-66-3

RX(3) OF B ...G + 2 K ==&gt; L

L2 ANSWER 12 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L

RX(3) RCT G 61010-04-6, K 146368-08-3

## STAGE(1)

RGT I 127-09-3 AcONa  
SOL 108-24-7 Ac2O  
CON 6 hours, room temperature

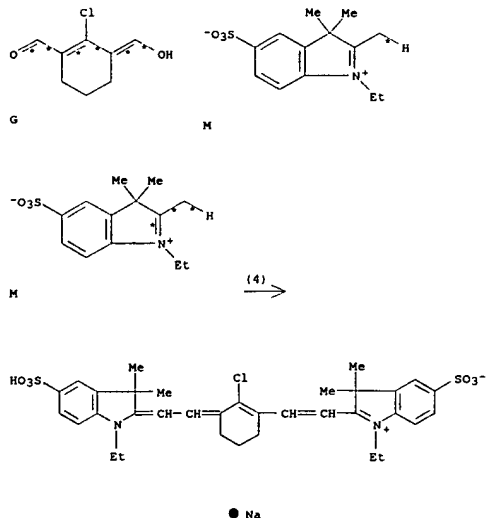
## STAGE(2)

RGT J 141-78-6 AcOEt  
CON room temperature

PRO L 749259-67-4

L2 ANSWER 12 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(4) OF B ...G + 2 M ==&gt; N



N

RX(4) RCT G 61010-04-6, M 146368-07-2

## STAGE(1)

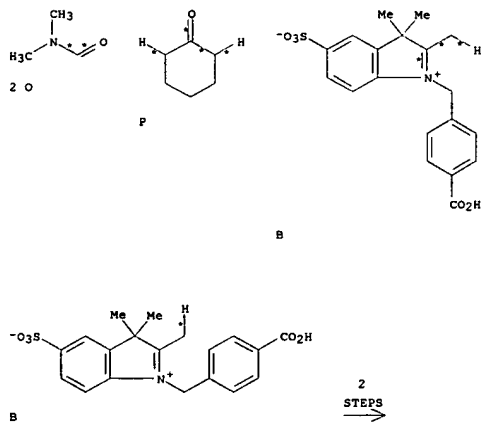
RGT I 127-09-3 AcONa  
SOL 108-24-7 Ac2O  
CON 6 hours, room temperature

## STAGE(2)

RGT J 141-78-6 AcOEt  
CON room temperature

PRO N 228717-21-3

L2 ANSWER 12 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(6) OF 8 COMPOSED OF RX(5), RX(2)  
RX(6) 2 O + P + 2 B ==> H

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT O 68-12-2, P 108-94-1  
RGT Q 10025-87-3 POCl3  
PRO G 61010-04-6  
SOL 75-09-2 CH2Cl2

RX(2) RCT G 61010-04-6, B 749259-68-5

## STAGE(1)

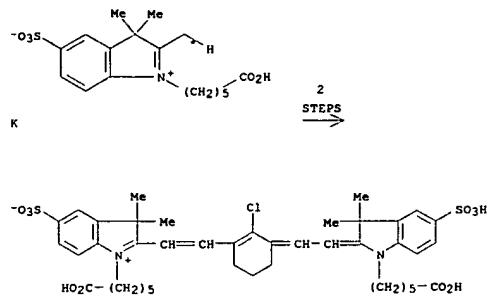
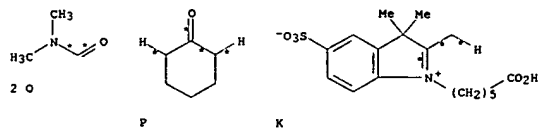
RGT I 127-09-3 AcONa  
SOL 108-24-7 Ac2O  
CON 6 hours, room temperature

## STAGE(2)

RGT J 141-78-6 AcOEt  
CON room temperature

PRO H 749259-66-3

L2 ANSWER 12 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 RX(7) OF 8 COMPOSED OF RX(5), RX(3)  
 RX(7) 2 O + P + 2 K ==> L



● Na  
 L  
 RX(5) RCT O 68-12-2, P 108-94-1  
 RGT Q 10025-87-3 POC13  
 PRO G 61010-04-6  
 SOL 75-09-2 CH2C12  
 RX(3) RCT G 61010-04-6, K 146368-08-3  
 STAGE(1)  
 RGT I 127-09-3 AcONa

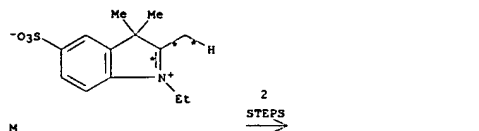
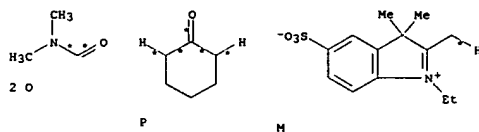
L2 ANSWER 12 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 RX(5) RCT O 68-12-2, P 108-94-1  
 RGT Q 10025-87-3 POC13  
 PRO G 61010-04-6  
 SOL 75-09-2 CH2C12  
 RX(4) RCT G 61010-04-6, M 146368-07-2  
 STAGE(1)  
 RGT I 127-09-3 AcONa  
 SOL 108-24-7 Ac2O  
 CON 6 hours, room temperature  
 STAGE(2)  
 RGT J 141-78-6 AcOEt  
 CON room temperature  
 PRO N 228717-21-3

L2 ANSWER 12 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 SOL 108-24-7 Ac2O  
 CON 6 hours, room temperature

STAGE(2)  
 RGT J 141-78-6 AcOEt  
 CON room temperature

PRO L 749259-67-4

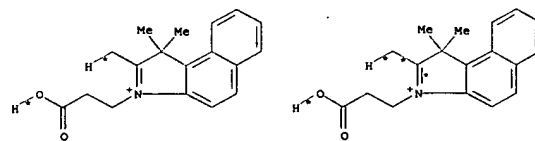
RX(8) OF 8 COMPOSED OF RX(5), RX(4)  
 RX(8) 2 O + P + 2 M ==> N



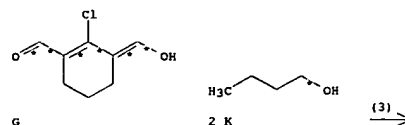
● Na  
 N

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 141:102606 CASREACT  
 TITLE: Synthesis and evaluation of polyhydroxylated near-infrared carbocyanine molecular probes  
 AUTHOR(S): Zhang, Zongren; Achilefu, Samuel  
 CORPORATE SOURCE: Department of Radiology, Washington University, St. Louis, MO, 63110, USA  
 SOURCE: Organic Letters (2004), 6(12), 2067-2070  
 CODEN: ORLE77; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A new near-IR (NIR) fluorescent mol. probe derived from indocarbocyanine dye and galactose was prepared, and the procedure was optimized. The presence of a nonionic polyhydroxyl moiety between hydrophobic groups enhances solubility and possibly minimizes aggregation in aqueous solns.  
 The structural framework of this mol. provides multivalent sites for labeling diverse mols.  
 REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(3) OF 26 ...2 C + G + 2 K ==> L...



● Br<sup>-</sup>  
 C

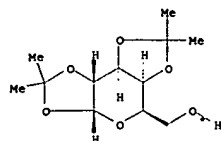


L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

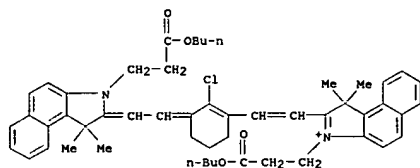
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(3) RCT C 415920-95-5, G 61010-04-6, K 71-36-3  
 PRO L 717901-33-2  
 SOL 71-43-2 Benzene, 71-36-3 BuOH  
 CON 15 hours, reflux  
 NTE product distribution depends on reaction conditions, optimization study, optimized on temperature, reaction time, solvent

RX(4) OF 26 ...N + L ==&gt; O...



N

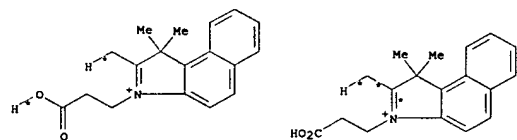
● Br<sup>-</sup>

(4) →

L

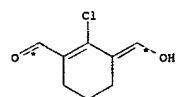
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● Br<sup>-</sup>● Br<sup>-</sup>

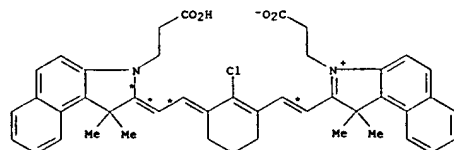
C

C



G

(5) →



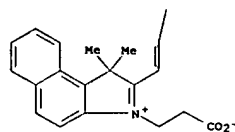
T

RX(5) RCT C 415920-95-5, G 61010-04-6  
 PRO T 193208-79-6  
 SOL 71-43-2 Benzene, 71-36-3 BuOH  
 CON 100 - 105 deg C  
 NTE product distribution depends on reaction conditions, alternate preparation also described

RX(6) OF 26 ...L ==&gt; T

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

O  
YIELD 37%

RX(4) RCT N 4064-06-6

STAGE(1)  
 RGT P 594-19-4 t-BuLi  
 SOL 109-99-9 THF, 109-66-0 Pentane  
 CON 30 minutes, room temperature

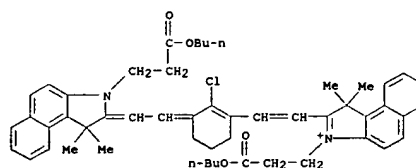
STAGE(2)  
 RCT L 717901-33-2  
 SOL 109-99-9 THF  
 CON 5 hours, room temperature

STAGE(3)  
 RGT Q 10035-10-6 HBr  
 SOL 7732-18-5 Water  
 CON room temperature, neutralized

PRO O 717901-34-3  
 NTE alternate preparation also described, other products also detected

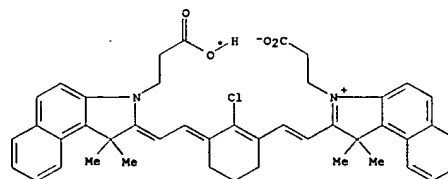
RX(5) OF 26 ...2 C + G ==&gt; T

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● Br<sup>-</sup>

L

(6) →

T  
YIELD 80%

RX(6) RCT L 717901-33-2  
 RGT U 865-48-5 NaOBu-t  
 PRO T 193208-79-6  
 SOL 109-99-9 THF  
 CON 24 hours, room temperature  
 NTE alternate preparation also described

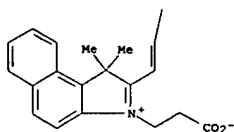
RX(7) OF 26 ...O ==&gt; V

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A



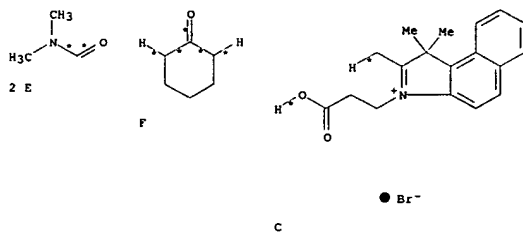
O

(7) →

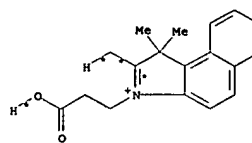
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(7) RCT O 717901-34-3  
 RGT M 76-05-1 F3CCO2H  
 PRO V 717901-32-1  
 CON 3 hours, room temperature

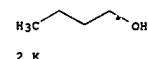
RX(10) OF 26 COMPOSED OF RX(2), RX(3)  
 RX(10) 2 E + F + 2 C + 2 K ==> L



L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



C

● Br<sup>-</sup>

2 K

2 STEPS →

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT E 68-12-2

STAGE(1)  
 RGT H 10025-87-3 POC13  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON 0 deg C

STAGE(2)  
 RCT F 108-94-1  
 CON SUBSTAGE(1) 2 hours, reflux  
 SUBSTAGE(2) reflux -> 0 deg C

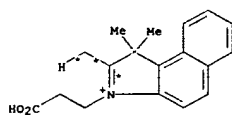
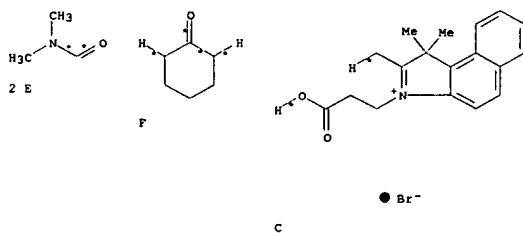
STAGE(3)  
 SOL 7732-18-5 Water  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 30 minutes, 0 deg C

PRO G 61010-04-6  
 NTE Vilsmeier reaction, regioselective

RX(3) RCT C 415920-95-5, G 61010-04-6, K 71-36-3  
 PRO L 717901-33-2  
 SOL 71-43-2 Benzene, 71-36-3 BuOH  
 CON 15 hours, reflux  
 NTE product distribution depends on reaction conditions, optimization study, optimized on temperature, reaction time, solvent

RX(11) OF 26 COMPOSED OF RX(2), RX(5)  
 RX(11) 2 E + F + 2 C ==> T

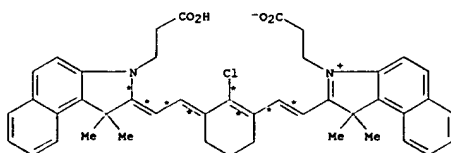
L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



C

● Br<sup>-</sup>

2 STEPS →



T

RX(2) RCT E 68-12-2

STAGE(1)  
 RGT H 10025-87-3 POC13

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON 0 deg C

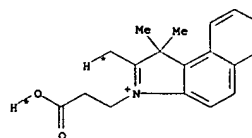
STAGE(2)  
 RCT F 108-94-1  
 CON SUBSTAGE(1) 2 hours, reflux  
 SUBSTAGE(2) reflux -> 0 deg C

STAGE(3)  
 SOL 7732-18-5 Water  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 30 minutes, 0 deg C

PRO G 61010-04-6  
 NTE Vilsmeier reaction, regioselective

RX(5) RCT C 415920-95-5, G 61010-04-6  
 PRO T 193208-79-6  
 SOL 71-43-2 Benzene, 71-36-3 BuOH  
 CON 100 - 105 deg C  
 NTE product distribution depends on reaction conditions, alternate preparation also described

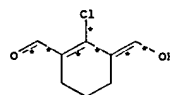
RX(12) OF 26 COMPOSED OF RX(3), RX(4)  
 RX(12) 2 C + G + 2 K + N ==> O



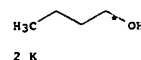
C

● Br<sup>-</sup>

C

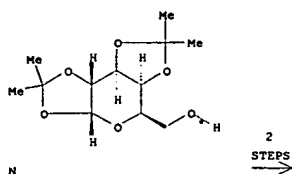
● Br<sup>-</sup>

G



2 K

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(3) RCT C 415920-95-5, G 61010-04-6, K 71-36-3  
 PRO L 717901-33-2  
 SOL 71-43-2 Benzene, 71-36-3 BuOH  
 CON 15 hours, reflux  
 NTE product distribution depends on reaction conditions, optimization study, optimized on temperature, reaction time, solvent

RX(4) RCT N 4064-06-6

STAGE(1)

RGT P 594-19-4 t-BuLi  
 SOL 109-99-9 THF, 109-66-0 Pentane  
 CON 30 minutes, room temperature

STAGE(2)

RCT L 717901-33-2  
 SOL 109-99-9 THF  
 CON 5 hours, room temperature

STAGE(3)

RGT Q 10035-10-6 HBr  
 SOL 7732-18-5 Water  
 CON room temperature, neutralized

PRO O 717901-34-3

NTE alternate preparation also described, other products also detected

RX(13) OF 26 COMPOSED OF RX(3), RX(6)

RX(13) 2 C + G + 2 K ==&gt; T

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 71-43-2 Benzene, 71-36-3 BuOH  
 CON 15 hours, reflux  
 NTE product distribution depends on reaction conditions, optimization study, optimized on temperature, reaction time, solvent

RX(6) RCT L 717901-33-2

RGT U 865-48-5 NaOBu-t

PRO T 193208-79-6

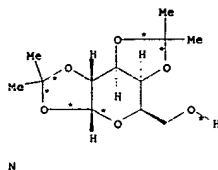
SOL 109-99-9 THF

CON 24 hours, room temperature

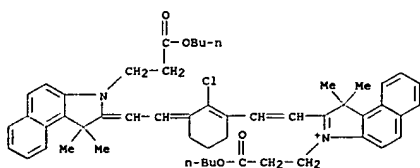
NTE alternate preparation also described

RX(14) OF 26 COMPOSED OF RX(4), RX(7)

RX(14) N + L ==&gt; V



N

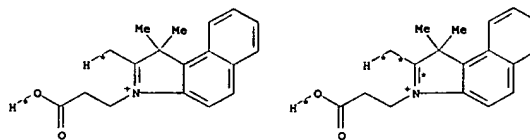
● Br<sup>-</sup>

L

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

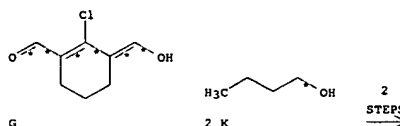
RX(4) RCT N 4064-06-6

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

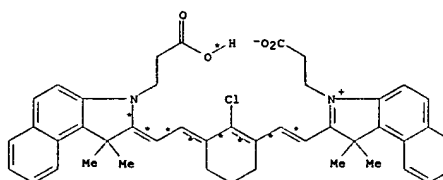


C

C



G

T  
YIELD 80%

RX(3) RCT C 415920-95-5, G 61010-04-6, K 71-36-3

PRO L 717901-33-2

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(1)

RGT P 594-19-4 t-BuLi  
 SOL 109-99-9 THF, 109-66-0 Pentane  
 CON 30 minutes, room temperature

STAGE(2)

RCT L 717901-33-2  
 SOL 109-99-9 THF  
 CON 5 hours, room temperature

STAGE(3)

RGT Q 10035-10-6 HBr  
 SOL 7732-18-5 Water  
 CON room temperature, neutralized

PRO O 717901-34-3

NTE alternate preparation also described, other products also detected

RX(7)

RCT O 717901-34-3

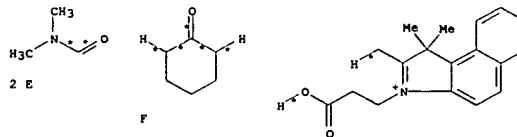
RGT W 76-05-1 F3CCO2H

PRO V 717901-32-1

CON 3 hours, room temperature

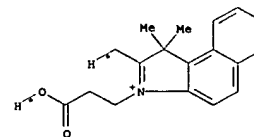
RX(19) OF 26 COMPOSED OF RX(2), RX(3), RX(4)

RX(19) 2 E + F + 2 C + 2 K + N ==&gt; O



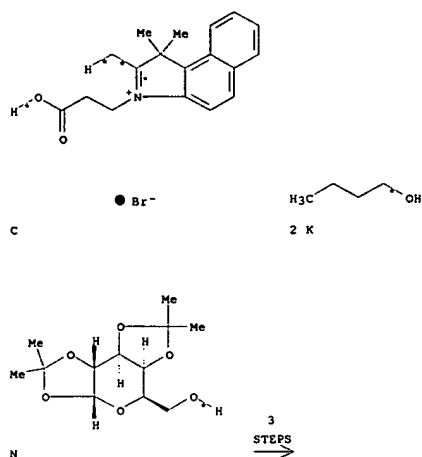
E

F

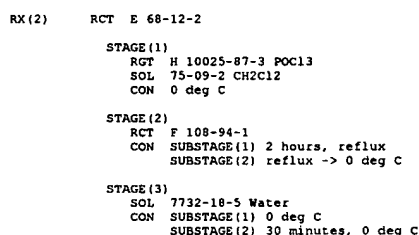


C

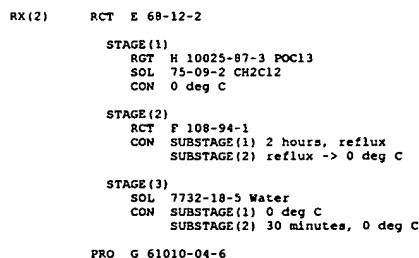
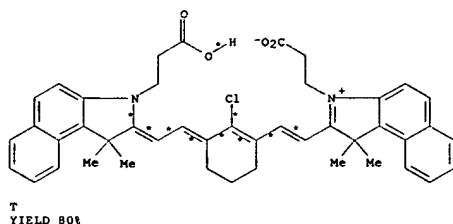
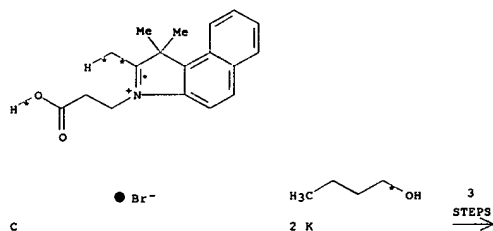
L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



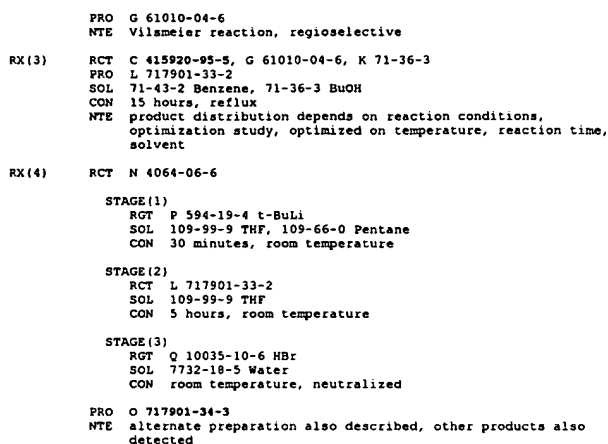
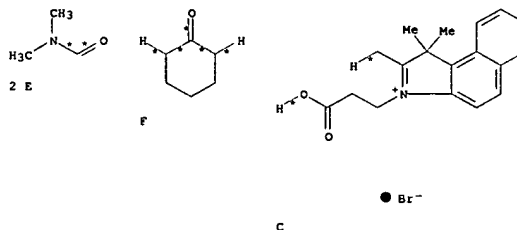
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



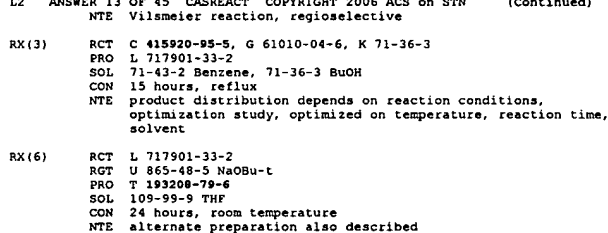
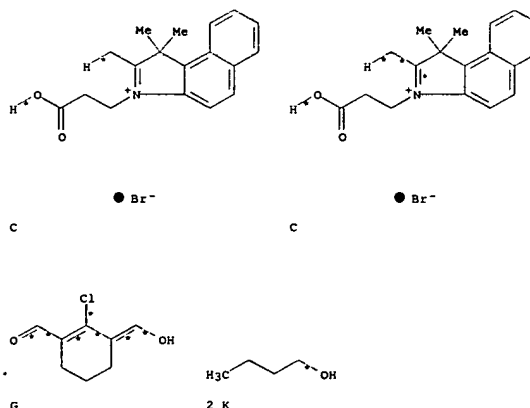
L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



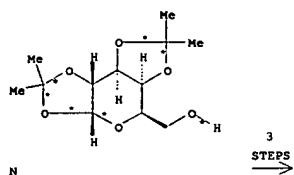
L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX (20) OF 26 COMPOSED OF RX (2), RX (3), RX (6)  
RX (20) 2 E + F + 2 C + 2 K  $\Rightarrow$  T

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX (21) OF 26 COMPOSED OF RX (3), RX (4), RX (7)  
RX (21) 2 C + G + 2 K + N  $\Rightarrow$  V

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(3) RCT C 415920-95-5, G 61010-04-6, K 71-36-3  
 PRO L 717901-33-2  
 SOL 71-43-2 Benzene, 71-36-3 BuOH  
 CON 15 hours, reflux  
 NTE product distribution depends on reaction conditions, optimization study, optimized on temperature, reaction time, solvent

RX(4) RCT N 4064-06-6

## STAGE(1)

RGT P 594-19-4 t-BuLi  
 SOL 109-99-9 THF, 109-66-0 Pentane  
 CON 30 minutes, room temperature

## STAGE(2)

RCT L 717901-33-2  
 SOL 109-99-9 THF  
 CON 5 hours, room temperature

## STAGE(3)

RGT Q 10035-10-6 HBr  
 SOL 7732-18-5 Water  
 CON room temperature, neutralized

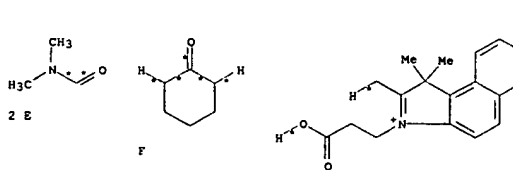
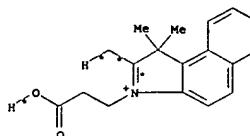
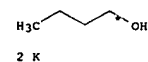
PRO O 717901-34-3

NTE alternate preparation also described, other products also detected

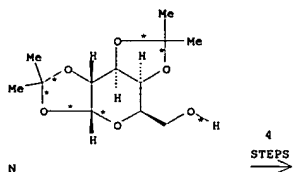
RX(7) RCT O 717901-34-3  
 RGT W 76-05-1 F3CCO2H  
 PRO V 717901-32-1  
 CON 3 hours, room temperature

RX(23) OF 26 COMPOSED OF RX(2), RX(3), RX(4), RX(7)

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● Br<sup>-</sup>● Br<sup>-</sup>

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT E 68-12-2

## STAGE(1)

RGT H 10025-87-3 POCl3  
 SOL 75-09-2 CH2Cl2  
 CON 0 deg C

## STAGE(2)

RCT F 108-94-1  
 CON SUBSTAGE(1) 2 hours, reflux  
 SUBSTAGE(2) reflux -> 0 deg C

## STAGE(3)

SOL 7732-18-5 Water  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 30 minutes, 0 deg C

PRO G 61010-04-6

NTE Vilsmeier reaction, regioselective

RX(3) RCT C 415920-95-5, G 61010-04-6, K 71-36-3  
 PRO L 717901-33-2  
 SOL 71-43-2 Benzene, 71-36-3 BuOH  
 CON 15 hours, reflux  
 NTE product distribution depends on reaction conditions, optimization study, optimized on temperature, reaction time, solvent

RX(4) RCT N 4064-06-6

## STAGE(1)

RGT P 594-19-4 t-BuLi  
 SOL 109-99-9 THF, 109-66-0 Pentane  
 CON 30 minutes, room temperature

## STAGE(2)

RCT L 717901-33-2  
 SOL 109-99-9 THF  
 CON 5 hours, room temperature

L2 ANSWER 13 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

## STAGE(3)

RGT Q 10035-10-6 HBr  
 SOL 7732-18-5 Water  
 CON room temperature, neutralized

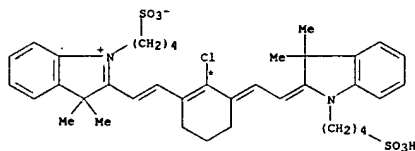
PRO O 717901-34-3

NTE alternate preparation also described, other products also detected

RX(7) RCT O 717901-34-3  
 RGT W 76-05-1 F3CCO2H  
 PRO V 717901-32-1  
 CON 3 hours, room temperature

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS ON STN  
 ACCESSION NUMBER: 141:72954 CASREACT  
 TITLE: Water-soluble pH-sensitive 2,6-bis(substituted ethylidene)-cyclohexanone/hydroxy cyanine dyes that absorb in the visible/near-infrared regions  
 AUTHOR(S): Strekowski, Lucjan; Mason, J. Christian; Lee, Hyeran; Say, Martial; Patonay, Gabor  
 CORPORATE SOURCE: Department of Chemistry, Georgia State University, Atlanta, GA, 30303, USA  
 SOURCE: Journal of Heterocyclic Chemistry (2004), 41(2), 227-232  
 CODEN: JHCTAD; ISSN: 0022-152X  
 PUBLISHER: HeteroCorporation  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Three methods were used to synthesize a series of the title compds. The ketones absorb in the visible region, and upon protonation (pH<6) they are converted to hydroxy-substituted heptamethine cyanines that show an intense absorption in the near-IR region (>700 nm). The conversion is reversible and depends solely on pH conditions.  
 REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS  
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(2) OF 30 E ==> F

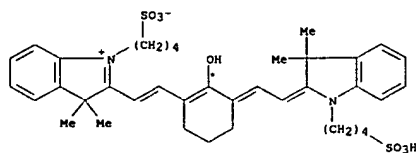


● Na

(2) →

E

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)



● Na

F  
YIELD 90%

RX(2) RCT E 115970-66-6

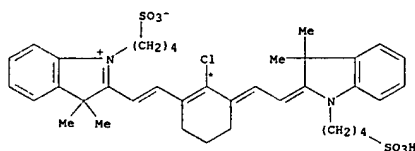
STAGE(1)  
 RGT G 127-09-3 AcONa  
 SOL 68-12-2 DMF  
 CON 3 hours, 80 deg C

STAGE(2)  
 RGT H 124-38-9 CO2  
 CON -78 deg C

PRO F 710337-86-3

RX(3) OF 30 E ==> F

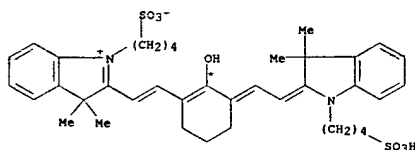
L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)



● Na

(3) →

E



● Na

F

RX(3) RCT E 115970-66-6

STAGE(1)  
 RGT J 124-41-4 NaOMe  
 SOL 67-56-1 MeOH  
 CON 8 hours, reflux

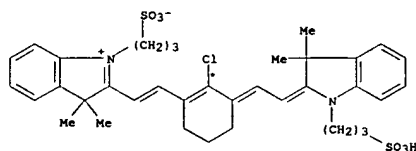
STAGE(2)  
 RGT H 124-38-9 CO2  
 CON -78 deg C

STAGE(3)  
 RGT K 7681-82-5 NaI  
 SOL 68-12-2 DMF  
 CON 12 hours, reflux

PRO F 710337-86-3

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)

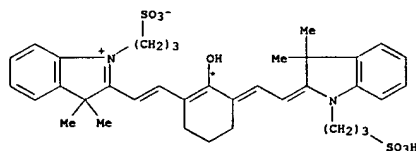
RX(4) OF 30 M ==> N



● Na

M

(4) →



● Na

N  
YIELD 90%

RX(4) RCT M 115970-63-3

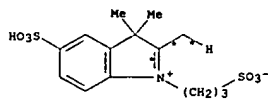
STAGE(1)  
 RGT G 127-09-3 AcONa  
 SOL 68-12-2 DMF  
 CON 3 hours, 80 deg C

STAGE(2)  
 RGT H 124-38-9 CO2  
 CON -78 deg C

PRO N 710337-87-4

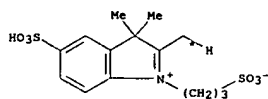
L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(5) OF 30 ...2 C + O ==&gt; P...



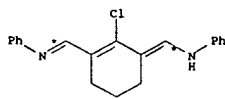
● Na

C



● Na

C

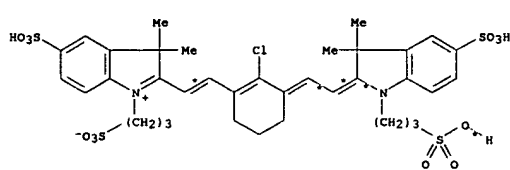


● HCl

O

(5) →

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



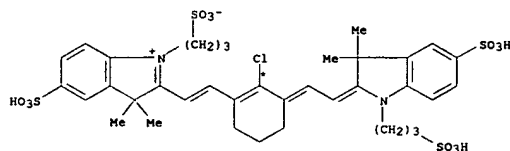
● 3 Na

P

YIELD 85%

RX(5) RCT C 407627-53-6, O 63857-00-1  
 RGT G 127-09-3 AcONa  
 PRO P 710337-84-1  
 SOL 64-17-5 EtOH  
 CON 2 - 5 hours, 80 deg C

RX(6) OF 30 ...P ==&gt; R

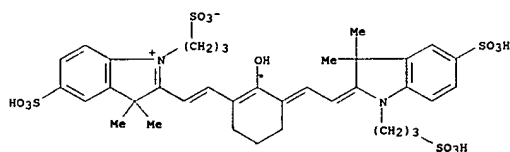


● 3 Na

P

(6) →

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

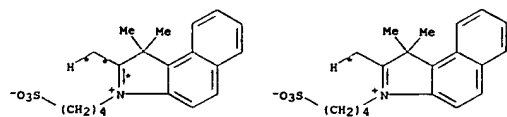


● 3 Na

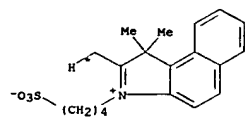
R

RX(6) RCT P 710337-84-1  
 STAGE(1)  
 RGT J 124-41-4 NaOMe  
 SOL 67-56-1 MeOH  
 CON 8 hours, reflux  
 STAGE(2)  
 RGT H 124-38-9 CO2  
 CON -78 deg C  
 STAGE(3)  
 RGT K 7681-82-5 NaI  
 SOL 68-12-2 DMF  
 CON 12 hours, reflux  
 PRO R 710337-88-5

RX(7) OF 30 2 S + O ==&gt; T...

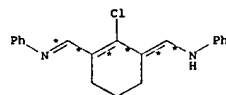


S



S

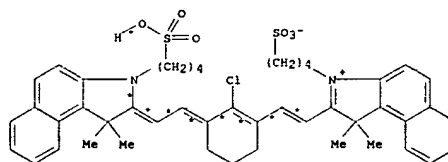
L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● HCl

O

(7) →



● Na

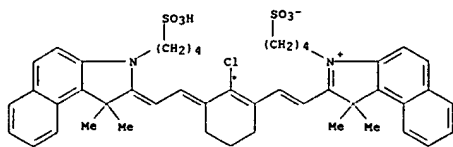
T

YIELD 90%

RX(7) RCT S 63149-24-6, O 63857-00-1  
 RGT G 127-09-3 AcONa  
 PRO T 172616-80-7  
 SOL 64-17-5 EtOH  
 CON 2 - 5 hours, 80 deg C

RX(8) OF 30 ...T ==&gt; U

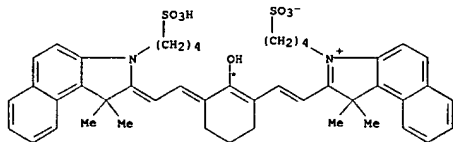
L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

T

(8) →



● Na

U

YIELD 90%

RX(8) RCT T 172616-80-7

STAGE(1)

RGT G 127-09-3 AcONa

SOL 68-12-2 DMF

CON 3 hours, 80 deg C

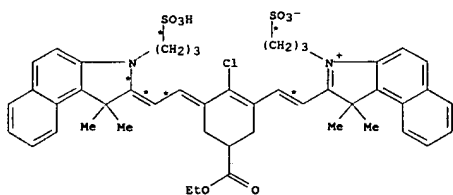
STAGE(2)

RGT H 124-38-9 CO2

CON -78 deg C

PRO U 710337-89-6

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

W

YIELD 97%

RX(9) RCT S 63149-24-6, V 710337-83-0

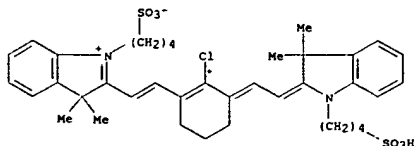
RGT G 127-09-3 AcONa

PRO W 215712-90-6

SOL 64-17-5 EtOH

CON 2 - 5 hours, 80 deg C

RX(10) OF 30 Z ==&gt; F



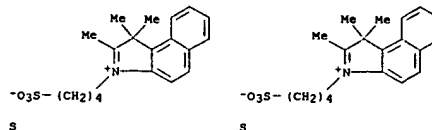
● Na

E

(10) →

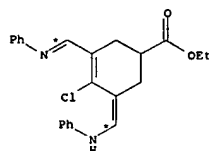
L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(9) OF 30 2 S + V ==&gt; W...



S

S

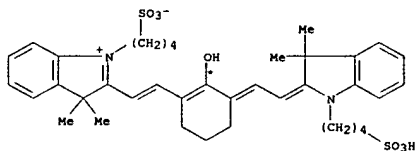


● HCl

V

(9) →

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

F

YIELD 90%

RX(10) RCT E 115970-66-6

STAGE(1)

RGT J 124-41-4 NaOMe

SOL 67-56-1 MeOH

CON 24 hours, reflux

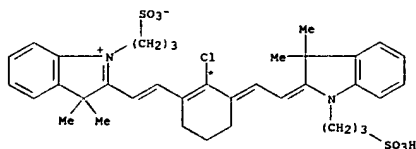
STAGE(2)

RGT H 124-38-9 CO2

CON -78 deg C

PRO F 710337-86-3

RX(11) OF 30 M ==&gt; N

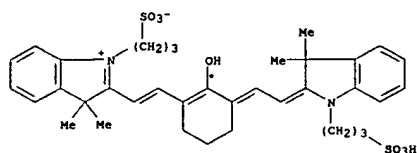


● Na

M

(11) →

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

N  
YIELD 90%

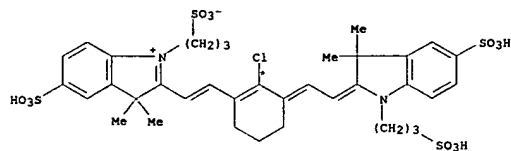
RX(11) RCT M 115970-63-3

STAGE(1)  
RGT J 124-41-4 NaOMe  
SOL 67-56-1 MeOH  
CON 24 hours, reflux

STAGE(2)  
RGT H 124-38-9 CO2  
CON -78 deg C

PRO N 710337-87-4

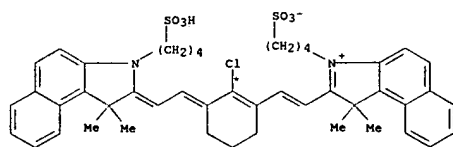
RX(12) OF 30 P ==&gt; R



● 3 Na

P

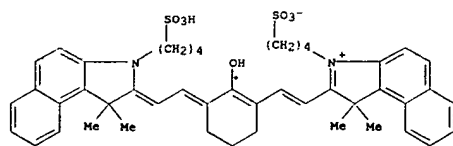
L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

T

(13) →



● Na

U  
YIELD 90%

RX(13) RCT T 172616-80-7

STAGE(1)  
RGT J 124-41-4 NaOMe  
SOL 67-56-1 MeOH  
CON 24 hours, reflux

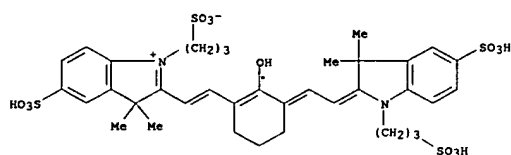
STAGE(2)  
RGT H 124-38-9 CO2  
CON -78 deg C

PRO U 710337-89-6

RX(14) OF 30 M + J ==&gt; X...

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

(12) →



● 3 Na

R  
YIELD 90%

RX(12) RCT P 710337-84-1

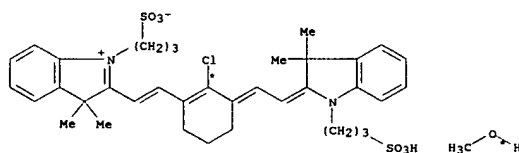
STAGE(1)  
RGT J 124-41-4 NaOMe  
SOL 67-56-1 MeOH  
CON 24 hours, reflux

STAGE(2)  
RGT H 124-38-9 CO2  
CON -78 deg C

PRO R 710337-88-5

RX(13) OF 30 T ==&gt; U

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



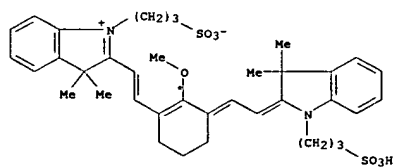
● Na

M

● Na

J

(14) →



● Na

X  
YIELD 80%

RX(14) RCT M 115970-63-3, J 124-41-4

STAGE(1)  
SOL 67-56-1 MeOH  
CON SUBSTAGE(1) 8 hours, reflux  
SUBSTAGE(2) room temperature

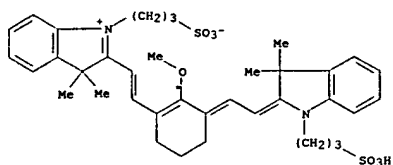
STAGE(2)  
RGT H 124-38-9 CO2  
CON -78 deg C

PRO X 710337-91-0



L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

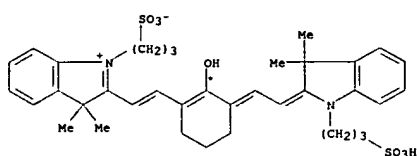
RX(15) OF 30 ...X ==&gt; N



● Na

X

(15)



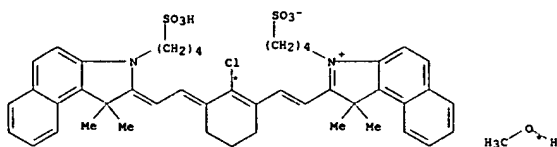
● Na

N  
YIELD 95%

RX(15) RCT X 710337-91-0  
RGT K 7681-82-5 NaI  
PRO N 710337-87-4  
SOL 68-12-2 DMF  
CON 12 hours, reflux

RX(16) OF 30 ...T + J ==&gt; Y...

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



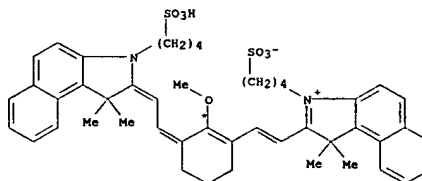
● Na

T

● Na

J

(16)



● Na

Y  
YIELD 87%

RX(16) RCT T 172616-80-7, J 124-41-4

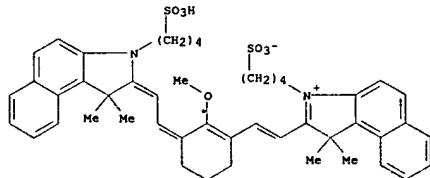
STAGE(1)  
SOL 67-56-1 MeOH  
CON SUBSTAGE(1) 8 hours, reflux  
SUBSTAGE(2) room temperature

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(2)  
RGT H 124-38-9 CO2  
CON -78 deg C

PRO Y 710337-93-2

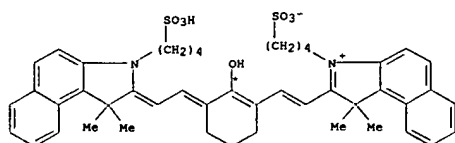
RX(17) OF 30 ...Y ==&gt; U



● Na

Y

(17)



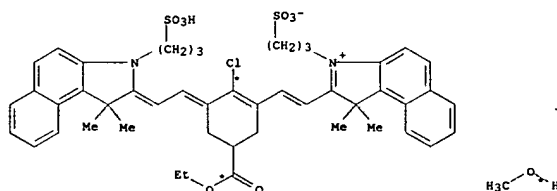
● Na

U  
YIELD 95%

RX(17) RCT Y 710337-93-2  
RGT K 7681-82-5 NaI  
PRO U 710337-89-6  
SOL 68-12-2 DMF  
CON 12 hours, reflux

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(18) OF 30 ...W + 2 J ==&gt; E...



● Na

W

● Na

2 J

(18)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(18) RCT W 215712-90-6, J 124-41-4

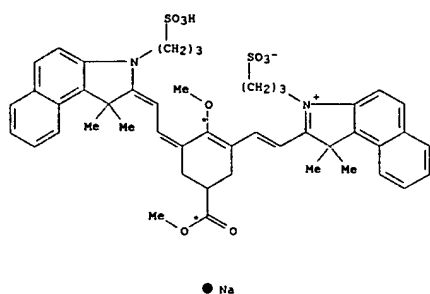
STAGE(1)  
SOL 67-56-1 MeOH  
CON SUBSTAGE(1) 8 hours, reflux  
SUBSTAGE(2) room temperature

STAGE(2)  
RGT H 124-38-9 CO2  
CON -78 deg C

PRO Z 710337-94-3

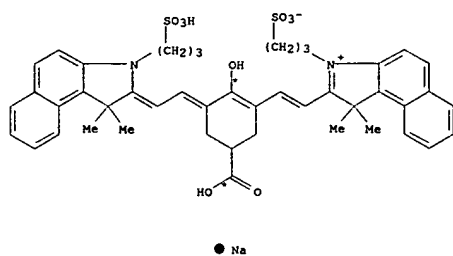
RX(19) OF 30 ...E ==&gt; AA

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



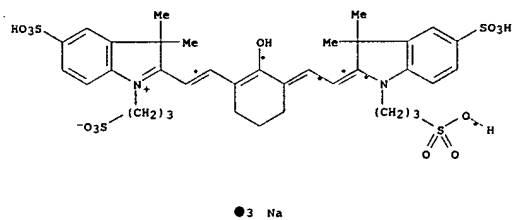
Z

(19)

AA  
YIELD 94%

RX(19) RCT Z 710337-94-3  
STAGE(1)  
RGT K 7681-82-5 NaI

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



R

RX(5) RCT C 407627-53-6, O 63857-00-1  
RGT G 127-09-3 AcONa  
PRO P 710337-84-1  
SOL 64-17-5 EtOH  
CON 2 - 5 hours, 80 deg C

RX(6) RCT P 710337-84-1  
STAGE(1)  
RGT J 124-41-4 NaOMe  
SOL 67-56-1 MeOH  
CON 8 hours, reflux  
STAGE(2)  
RGT H 124-38-9 CO2  
CON -78 deg C  
STAGE(3)  
RGT K 7681-82-5 NaI  
SOL 68-12-2 DMF  
CON 12 hours, reflux  
PRO R 710337-88-5

RX(22) OF 30 COMPOSED OF RX(7), RX(8)  
RX(22) 2 S + O ==> U

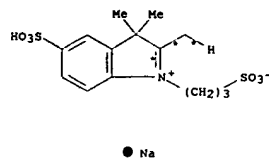
L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 68-12-2 DMF  
CON 12 hours, 80 deg C

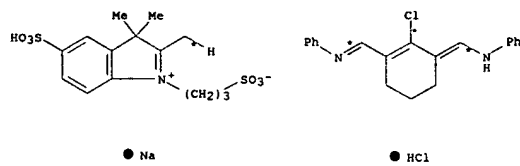
STAGE(2)  
RGT H 124-38-9 CO2  
CON -78 deg C

PRO AA 710337-95-4

RX(21) OF 30 COMPOSED OF RX(5), RX(6)  
RX(21) 2 C + O ==> R



C

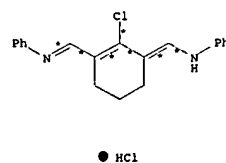
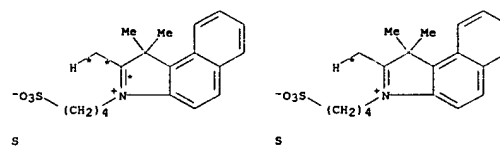


C

O

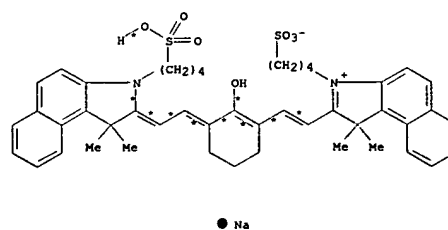
2  
STEPS

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



O

2  
STEPS

U  
YIELD 90%

RX(7) RCT S 63149-24-6, O 63857-00-1  
RGT G 127-09-3 AcONa  
PRO T 172616-80-7  
SOL 64-17-5 EtOH  
CON 2 - 5 hours, 80 deg C

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

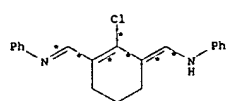
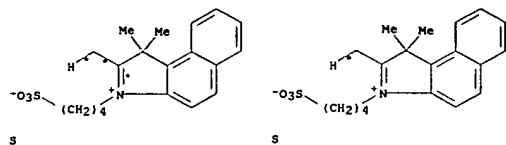
RX(8) RCT T 172616-80-7

STAGE(1)  
 RGT G 127-09-3 AcONa  
 SOL 68-12-2 DMF  
 CON 3 hours, 80 deg C

STAGE(2)  
 RGT H 124-38-9 CO2  
 CON -78 deg C

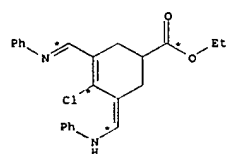
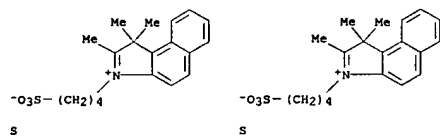
PRO U 710337-89-6

RX(23) OF 30 COMPOSED OF RX(7), RX(16)  
 RX(23) 2 S + O + J ==> Y



2  
 STEPS

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



2  
 STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(9) RCT S 63149-24-6, V 710337-83-0  
 RGT G 127-09-3 AcONa  
 PRO W 215712-90-6  
 SOL 64-17-5 EtOH  
 CON 2 - 5 hours, 80 deg C

RX(18) RCT W 215712-90-6, J 124-41-4

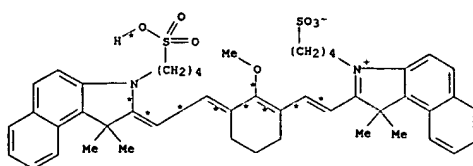
STAGE(1)  
 SOL 67-56-1 MeOH  
 CON SUBSTAGE(1) 8 hours, reflux  
 SUBSTAGE(2) room temperature

STAGE(2)  
 RGT H 124-38-9 CO2  
 CON -78 deg C

PRO Z 710337-94-3

RX(25) OF 30 COMPOSED OF RX(14), RX(15)  
 RX(25) M + J ==> N

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

Y  
 YIELD 87%

RX(7) RCT S 63149-24-6, O 63857-00-1  
 RGT G 127-09-3 AcONa  
 PRO T 172616-80-7  
 SOL 64-17-5 EtOH  
 CON 2 - 5 hours, 80 deg C

RX(16) RCT T 172616-80-7, J 124-41-4

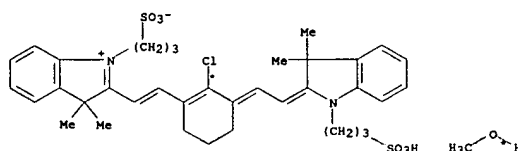
STAGE(1)  
 SOL 67-56-1 MeOH  
 CON SUBSTAGE(1) 8 hours, reflux  
 SUBSTAGE(2) room temperature

STAGE(2)  
 RGT H 124-38-9 CO2  
 CON -78 deg C

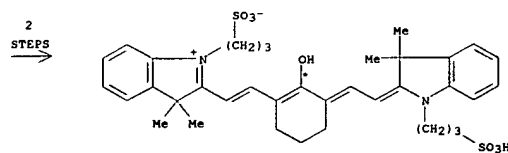
PRO Y 710337-93-2

RX(24) OF 30 COMPOSED OF RX(9), RX(18)  
 RX(24) 2 S + V + 2 J ==> E

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



2  
 STEPS



● Na

N  
 YIELD 95%

RX(14) RCT M 115970-63-3, J 124-41-4

STAGE(1)  
 SOL 67-56-1 MeOH  
 CON SUBSTAGE(1) 8 hours, reflux  
 SUBSTAGE(2) room temperature

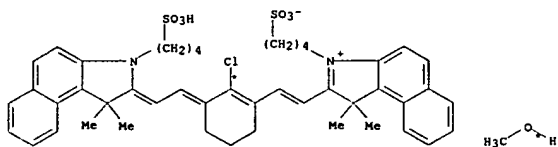
STAGE(2)  
 RGT H 124-38-9 CO2  
 CON -78 deg C

PRO X 710337-91-0

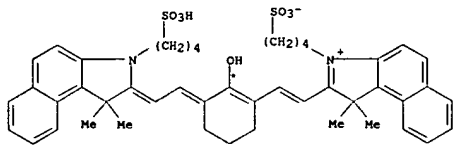
RX(15) RCT X 710337-91-0  
 RGT K 7681-82-5 NaI

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 PRO N 710337-87-4  
 SOL 68-12-2 DMF  
 CON 12 hours, reflux

RX(26) OF 30 COMPOSED OF RX(16), RX(17)  
 RX(26) T + J ==> U



2  
STEPS

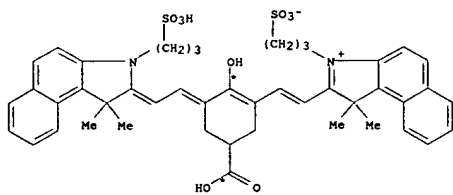


U  
YIELD 95%

RX(16) RCT T 172616-80-7, J 124-41-4  
 STAGE(1)  
 SOL 67-56-1 MeOH

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

2  
STEPS



AA  
YIELD 94%

RX(18) RCT W 215712-90-6, J 124-41-4  
 STAGE(1)  
 SOL 67-56-1 MeOH  
 CON SUBSTAGE(1) 8 hours, reflux  
 SUBSTAGE(2) room temperature

STAGE(2)  
 RGT H 124-38-9 CO<sub>2</sub>  
 CON -78 deg C

PRO Z 710337-94-3

RX(19) RCT Z 710337-94-3  
 STAGE(1)  
 RGT K 7681-82-5 NaI  
 SOL 68-12-2 DMF  
 CON 12 hours, 80 deg C

STAGE(2)  
 RGT H 124-38-9 CO<sub>2</sub>  
 CON -78 deg C

PRO AA 710337-95-4

RX(29) OF 30 COMPOSED OF RX(7), RX(16), RX(17)  
 RX(29) 2 S + O + J ==> U

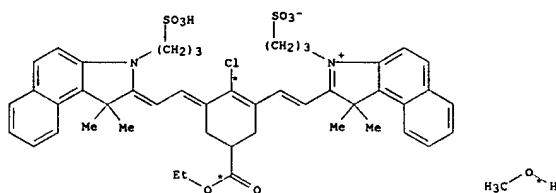
L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 CON SUBSTAGE(1) 8 hours, reflux  
 SUBSTAGE(2) room temperature

STAGE(2)  
 RGT H 124-38-9 CO<sub>2</sub>  
 CON -78 deg C

PRO Y 710337-93-2

RX(17) RCT Y 710337-93-2  
 RGT K 7681-82-5 NaI  
 PRO U 710337-89-6  
 SOL 68-12-2 DMF  
 CON 12 hours, reflux

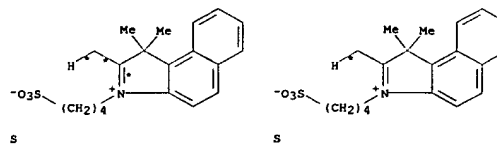
RX(27) OF 30 COMPOSED OF RX(18), RX(19)  
 RX(27) W + 2 J ==> AA



W

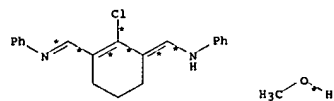
2 J

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



S

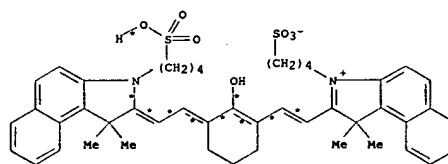
S



O

J

3  
STEPS



U

YIELD 95%

RX(7) RCT S 63149-24-6, O 63857-00-1  
 RGT G 127-09-3 AcONa  
 PRO T 172616-80-7  
 SOL 64-17-5 EtOH  
 CON 2 - 5 hours, 80 deg C

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(16) RCT T 172616-80-7, J 124-41-4

## STAGE(1)

SOL 67-56-1 MeOH  
CON SUBSTAGE(1) 8 hours, reflux  
SUBSTAGE(2) room temperature

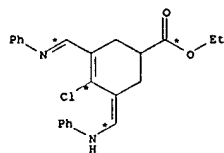
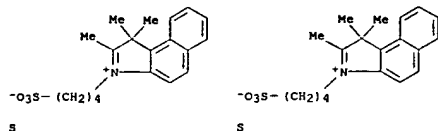
## STAGE(2)

RGT H 124-38-9 CO<sub>2</sub>  
CON -78 deg C

PRO Y 710337-93-2

RX(17) RCT Y 710337-93-2  
RGT K 7681-82-5 NaI  
PRO U 710337-89-6  
SOL 68-12-2 DMF  
CON 12 hours, reflux

RX(30) OF 30 COMPOSED OF RX(9), RX(18), RX(19)  
RX(30) 2 S + V + 2 J ==> AA



● HCl

● Na

3

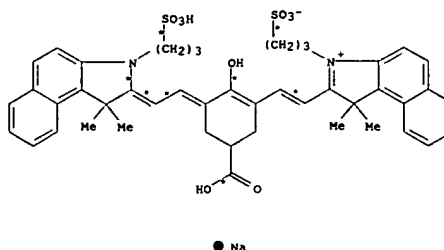
STEPS

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

CON -78 deg C

PRO AA 710337-95-4

L2 ANSWER 14 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

AA  
YIELD 94%

RX(9) RCT S 63149-24-6, V 710337-83-0  
RGT G 127-09-3 AcONa  
PRO W 215712-90-6  
SOL 64-17-5 EtOH  
CON 2 - 5 hours, 80 deg C

RX(18) RCT W 215712-90-6, J 124-41-4

## STAGE(1)

SOL 67-56-1 MeOH  
CON SUBSTAGE(1) 8 hours, reflux  
SUBSTAGE(2) room temperature

## STAGE(2)

RGT H 124-38-9 CO<sub>2</sub>  
CON -78 deg C

PRO Z 710337-94-3

RX(19) RCT Z 710337-94-3

## STAGE(1)

RGT K 7681-82-5 NaI  
SOL 68-12-2 DMF  
CON 12 hours, 80 deg C

## STAGE(2)

RGT H 124-38-9 CO<sub>2</sub>

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 140:78503 CASREACT  
TITLE: Synthesis and optical recording properties of some novel styryl dyes for DVD-R  
AUTHOR(S): Lee, Chung-Chun; Hu, Andrew Teh  
CORPORATE SOURCE: Department of Chemical Engineering, National Tsing Hua University, Hsin-Chu, Taiwan

SOURCE: Dyes and Pigments (2003), 59(1), 63-69  
CODEN: DYPIPX; ISSN: 0143-7208  
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis and spectral properties of styryl dyes having julolidinyl derivative moieties at one side of the styryl dye structure are described.

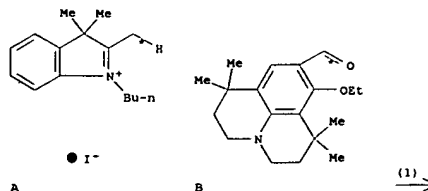
These dyes are designed to have different side groups with either carboxylate, ether, or sulfonate linkages on the julolidinyl ring. Differences in optical, thermal, and optical recording properties between these dyes have been compared. The relationships between the side groups and optical/thermal properties of the dyes are discussed.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS

FORMAT

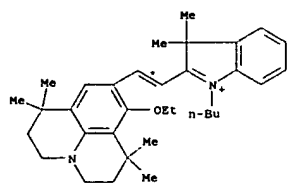
RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(1) OF 63 ...A + B ==&gt; C



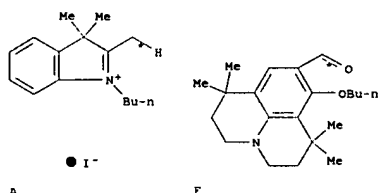
L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

● I<sup>-</sup>C  
YIELD 75%

RX(1) RCT A 20205-30-5, B 639818-47-6  
 RGT D 110-86-1 Pyridine  
 PRO C 639818-43-2  
 SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

RX(2) OF 63 ...A + F ==&gt; G

● I<sup>-</sup>

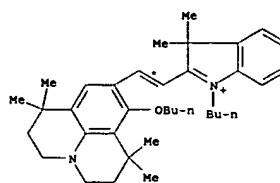
A

F

(2) →

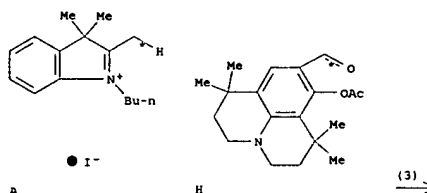
L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

● I<sup>-</sup>G  
YIELD 71%

RX(2) RCT A 20205-30-5, F 639818-48-7  
 RGT D 110-86-1 Pyridine  
 PRO G 639818-44-3  
 SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

RX(3) OF 63 ...A + H ==&gt; I

● I<sup>-</sup>

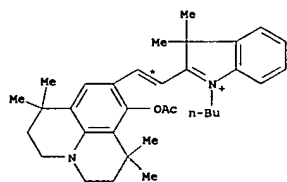
A

H

(3) →

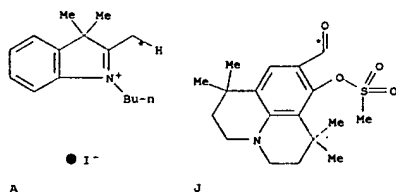
L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

● I<sup>-</sup>I  
YIELD 66%

RX(3) RCT A 20205-30-5, H 639818-49-8  
 RGT D 110-86-1 Pyridine  
 PRO I 639818-45-4  
 SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

RX(4) OF 63 ...A + J ==&gt; K

● I<sup>-</sup>

A

J

(4) →

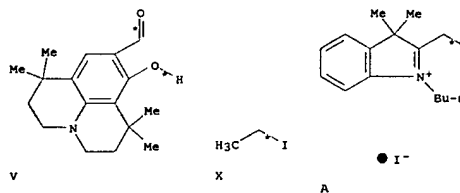
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(4) RCT A 20205-30-5, J 639818-50-1  
 RGT D 110-86-1 Pyridine  
 PRO K 639818-46-5  
 SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

RX(19) OF 63 COMPOSED OF RX(8), RX(1)  
 RX(19) V + X + A ==> C



V

X

A

● I<sup>-</sup>2  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(8) RCT V 115662-09-4

STAGE(1)  
 RGT Y 7646-69-7 NaH  
 SOL 68-12-2 DMF  
 CON 2 hours, room temperature

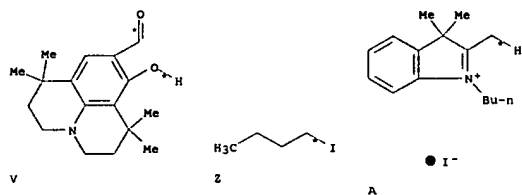
STAGE(2)  
 RCT X 75-03-6  
 CON 12 hours, room temperature

PRO B 639818-47-6

RX(1) RCT A 20205-30-5, B 639818-47-6  
 RGT D 110-86-1 Pyridine  
 PRO C 639818-43-2  
 SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

RX(20) OF 63 COMPOSED OF RX(9), RX(2)  
 RX(20) V + 2 + A ==> G

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



2  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(9)     RCT V 115662-09-4

STAGE(1)

RGT Y 7646-69-7 NaH

SOL 68-12-2 DMF

CON 2 hours, room temperature

STAGE(2)

RCT Z 542-69-8

CON 12 hours, room temperature

PRO F 639818-48-7

RX(2)     RCT A 20205-30-5, F 639818-48-7

RGT D 110-86-1 Pyridine

PRO G 639818-44-3

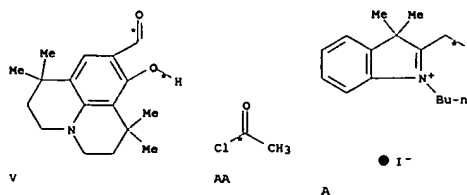
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-

CON overnight, reflux

RX(21) OF 63 COMPOSED OF RX(10), RX(3)

RX(21)     V + AA + A ==> I

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



2  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(10)     RCT V 115662-09-4, AA 75-36-5

RGT AB 121-44-8 Et3N

PRO H 639818-49-8

SOL 67-66-3 CHCl3

CON 4 hours, room temperature

RX(3)     RCT A 20205-30-5, H 639818-49-8

RGT D 110-86-1 Pyridine

PRO I 639818-45-4

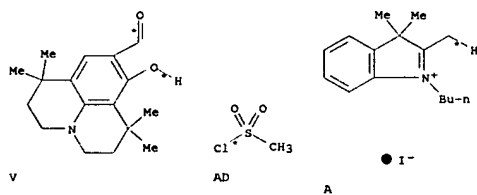
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-

CON overnight, reflux

RX(22) OF 63 COMPOSED OF RX(11), RX(4)

RX(22)     V + AD + A ==> K

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



2  
STEPS  
→

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(11)     RCT V 115662-09-4, AD 124-63-0

RGT AB 121-44-8 Et3N

PRO J 639818-50-1

SOL 67-66-3 CHCl3

CON 4 hours, room temperature

RX(4)     RCT A 20205-30-5, J 639818-50-1

RGT D 110-86-1 Pyridine

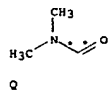
PRO K 639818-46-5

SOL 1320-67-8 Propanol, 1(or 2)-methoxy-

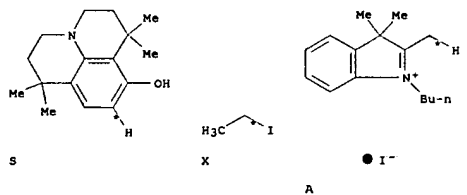
CON overnight, reflux

RX(36) OF 63 COMPOSED OF RX(7), RX(8), RX(1)

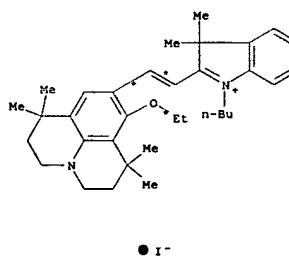
RX(36)     Q + S + X + A ==> C



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



3  
STEPS  
→



YIELD 75%

RX(7)     RCT Q 68-12-2

STAGE(1)

RGT W 10025-87-3 POC13

SOL 68-12-2 DMF

CON 2 hours, 0 deg C

STAGE(2)

RCT S 115704-83-1

SOL 68-12-2 DMF

CON 12 hours, room temperature

STAGE(3)

RGT O 127-09-3 AcONa

SOL 7732-18-5 Water

CON overnight, 0 deg C, pH 7 - 8

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

RX(8) RCT V 115662-09-4

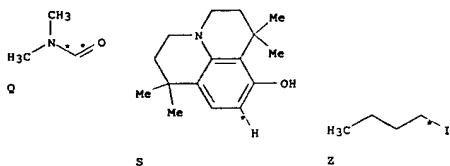
STAGE(1)  
RGT Y 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT X 75-03-6  
CON 12 hours, room temperature

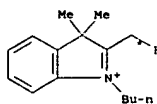
PRO B 639818-47-6

RX(1) RCT A 20205-30-5, B 639818-47-6  
RGT D 110-86-1 Pyridine  
PRO C 639818-43-2  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(37) OF 63 COMPOSED OF RX(7), RX(9), RX(2)  
RX(37) Q + S + Z + A ==> G



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(7) RCT Q 68-12-2

STAGE(1)  
RGT W 10025-87-3 POC13  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

RX(9) RCT V 115662-09-4

STAGE(1)  
RGT Y 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT Z 542-69-8  
CON 12 hours, room temperature

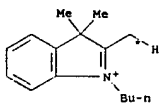
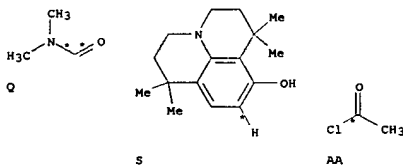
PRO F 639818-48-7

RX(2) RCT A 20205-30-5, F 639818-48-7

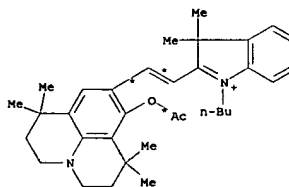
L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RGT D 110-86-1 Pyridine  
PRO G 639818-44-3  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(38) OF 63 COMPOSED OF RX(7), RX(10), RX(3)  
RX(38) Q + S + AA + A ==> I



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

I  
YIELD 66%

RX(7) RCT Q 68-12-2

STAGE(1)  
RGT W 10025-87-3 POC13  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

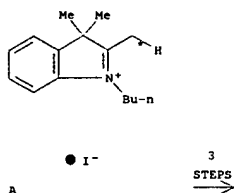
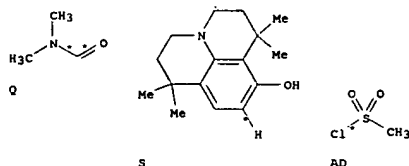
RX(10) RCT V 115662-09-4, AA 75-36-5  
RGT AB 121-44-8 Et3N  
PRO H 639818-49-8  
SOL 67-66-3 CHCl3  
CON 4 hours, room temperature

RX(3) RCT A 20205-30-5, H 639818-49-8  
RGT D 110-86-1 Pyridine  
PRO I 639818-45-4  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(39) OF 63 COMPOSED OF RX(7), RX(11), RX(4)



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
RX(39) Q + S + AD + A ==> K



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

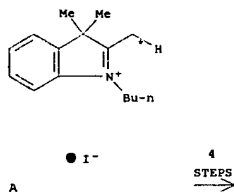
RX(7) RCT Q 68-12-2

STAGE(1)  
RGT W 10025-87-3 POCl3  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(6) RCT N 115662-07-2

STAGE(1)  
RGT T 75-75-2 MeSO3H  
CON 2 hours, 95 deg C

STAGE(2)  
RGT U 1336-21-6 NH4OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

STAGE(1)  
RGT W 10025-87-3 POCl3  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

RX(8) RCT V 115662-09-4

STAGE(1)  
RGT Y 7646-69-7 NaH  
SOL 68-12-2 DMF

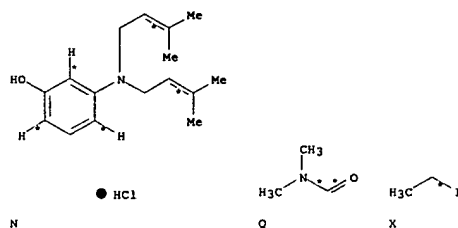
L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

RX(11) RCT V 115662-09-4, AD 124-63-0  
RGT AB 121-44-8 Et3N  
PRO J 639818-50-1  
SOL 67-66-3 CHCl3  
CON 4 hours, room temperature

RX(4) RCT A 20205-30-5, J 639818-50-1  
RGT D 110-86-1 Pyridine  
PRO K 639818-46-5  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(40) OF 63 COMPOSED OF RX(6), RX(7), RX(8), RX(1)  
RX(40) N + Q + X + A ==> C



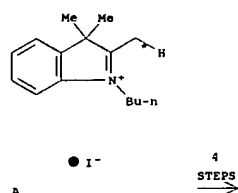
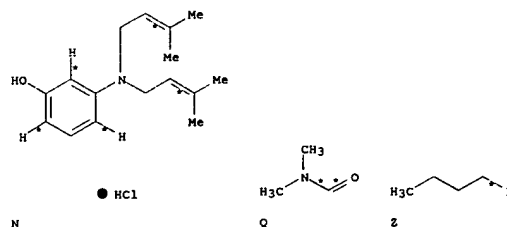
L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(2)  
RCT X 75-03-6  
CON 12 hours, room temperature

PRO B 639818-47-6

RX(1) RCT A 20205-30-5, B 639818-47-6  
RGT D 110-86-1 Pyridine  
PRO C 639818-43-2  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(41) OF 63 COMPOSED OF RX(6), RX(7), RX(9), RX(2)  
RX(41) N + Q + Z + A ==> G



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
RX(6) RCT N 115662-07-2

STAGE(1)  
RGT T 75-75-2 MeSO<sub>3</sub>H  
CON 2 hours, 95 deg C

STAGE(2)  
RGT U 1336-21-6 NH<sub>4</sub>OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

STAGE(1)  
RGT W 10025-87-3 POCl<sub>3</sub>  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

RX(9) RCT V 115662-09-4

STAGE(1)  
RGT Y 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

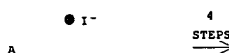
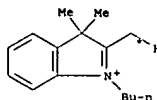
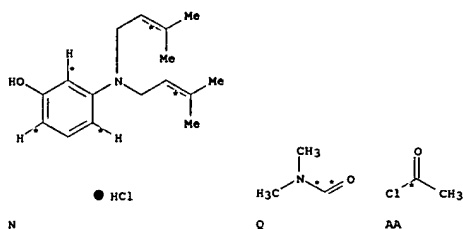
STAGE(2)  
RCT Z 542-69-8  
CON 12 hours, room temperature

PRO F 639818-48-7

RX(2) RCT A 20205-30-5, F 639818-48-7  
RGT D 110-86-1 Pyridine  
PRO G 639818-44-3  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(42) OF 63 COMPOSED OF RX(6), RX(7), RX(10), RX(3)  
RX(42) N + Q + AA + A ==> I

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(6) RCT N 115662-07-2

STAGE(1)  
RGT T 75-75-2 MeSO<sub>3</sub>H  
CON 2 hours, 95 deg C

STAGE(2)  
RGT U 1336-21-6 NH<sub>4</sub>OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(7) RCT Q 68-12-2

STAGE(1)  
RGT W 10025-87-3 POCl<sub>3</sub>  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

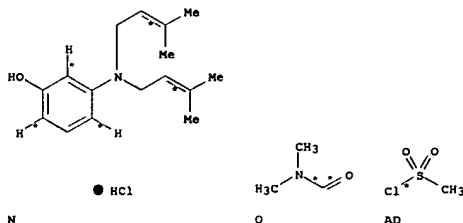
STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

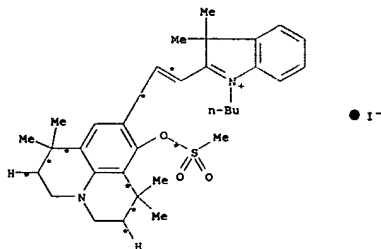
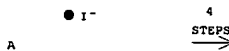
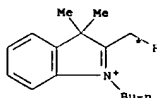
RX(10) RCT V 115662-09-4, AA 75-36-5  
RGT AB 121-44-8 Et<sub>3</sub>N  
PRO H 639818-49-8  
SOL 67-66-3 CHCl<sub>3</sub>  
CON 4 hours, room temperature

RX(3) RCT A 20205-30-5, H 639818-49-8  
RGT D 110-86-1 Pyridine  
PRO I 639818-45-4  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(43) OF 63 COMPOSED OF RX(6), RX(7), RX(11), RX(4)  
RX(43) N + Q + AD + A ==> K



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



K  
YIELD 74%

RX(6) RCT N 115662-07-2

STAGE(1)  
RGT T 75-75-2 MeSO<sub>3</sub>H  
CON 2 hours, 95 deg C

STAGE(2)  
RGT U 1336-21-6 NH<sub>4</sub>OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

STAGE(1)

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 RGT W 10025-87-3 POCl3  
 SOL 68-12-2 DMF  
 CON 2 hours, 0 deg C

STAGE(2)  
 RCT S 115704-83-1  
 SOL 68-12-2 DMF  
 CON 12 hours, room temperature

STAGE(3)  
 RGT O 127-09-3 AcONa  
 SOL 7732-18-5 Water  
 CON overnight, 0 deg C, pH 7 - 8

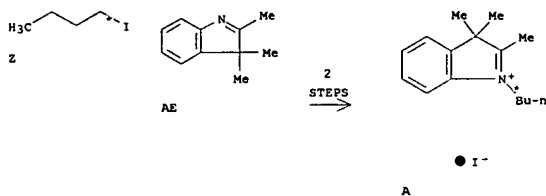
PRO V 115662-09-4  
 NTE Vilsmeier-Haak reaction

RX(11) RCT V 115662-09-4, AD 124-63-0  
 RGT AB 121-44-8 Et3N  
 PRO J 639818-50-1  
 SOL 67-66-3 CHCl3  
 CON 4 hours, room temperature

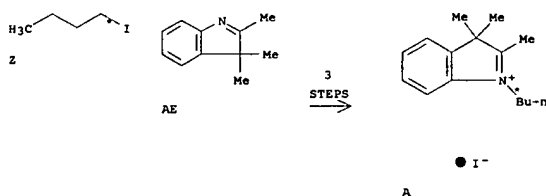
RX(4) RCT A 20205-30-5, J 639818-50-1  
 RGT D 110-86-1 Pyridine  
 PRO K 639818-46-5  
 SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

RX(44) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(1)  
 AND REACTION SEQUENCE RX(8), RX(1)

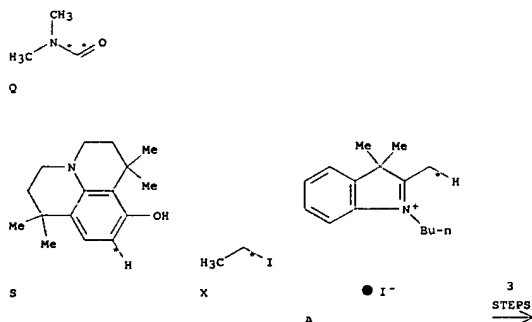
...Z + AE ==> A...  
 ...V + X + A ==> C



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 ...Q + S + X + A ==> C



START NEXT REACTION SEQUENCE



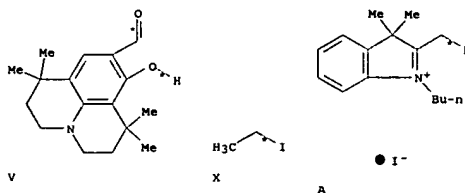
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
 RGT D 110-86-1 Pyridine  
 PRO A 20205-30-5  
 SOL 78-93-3 EtCOMe  
 CON 6 hours, reflux

RX(17) RCT Q 68-12-2

STAGE(1)  
 RGT W 10025-87-3 POCl3  
 SOL 68-12-2 DMF

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



2  
 STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
 RGT D 110-86-1 Pyridine  
 PRO A 20205-30-5  
 SOL 78-93-3 EtCOMe  
 CON 6 hours, reflux

RX(8) RCT V 115662-09-4

STAGE(1)  
 RGT Y 7646-69-7 NaH  
 SOL 68-12-2 DMF  
 CON 2 hours, room temperature

STAGE(2)  
 RCT X 75-03-6  
 CON 12 hours, room temperature

PRO B 639818-47-6

RX(1) RCT A 20205-30-5, B 639818-47-6  
 RGT D 110-86-1 Pyridine  
 PRO C 639818-43-2  
 SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

RX(45) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(1)  
 AND REACTION SEQUENCE RX(7), RX(8), RX(1)

...Z + AE ==> A...

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 CON 2 hours, 0 deg C

STAGE(2)  
 RCT S 115704-83-1  
 SOL 68-12-2 DMF  
 CON 12 hours, room temperature

STAGE(3)  
 RGT O 127-09-3 AcONa  
 SOL 7732-18-5 Water  
 CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
 NTE Vilsmeier-Haak reaction

RX(8) RCT V 115662-09-4

STAGE(1)  
 RGT Y 7646-69-7 NaH  
 SOL 68-12-2 DMF  
 CON 2 hours, room temperature

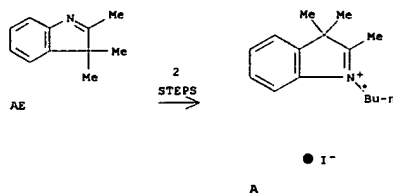
STAGE(2)  
 RCT X 75-03-6  
 CON 12 hours, room temperature

PRO B 639818-47-6

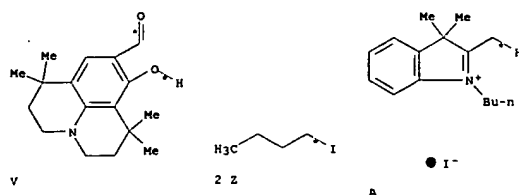
RX(1) RCT A 20205-30-5, B 639818-47-6  
 RGT D 110-86-1 Pyridine  
 PRO C 639818-43-2  
 SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

RX(46) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(2)  
 AND REACTION SEQUENCE RX(9), RX(2)

...Z + AE ==> A...  
 ...V + Z + A ==> G



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

2  
STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
RGT D 110-86-1 Pyridine  
PRO A 20205-30-5  
SOL 78-93-3 EtOMe  
CON 6 hours, reflux

RX(9) RCT V 115662-09-4

STAGE(1)  
RGT Y 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

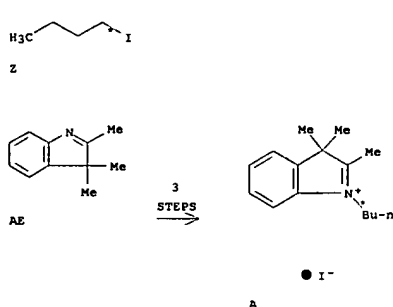
STAGE(2)  
RCT Z 542-69-8  
CON 12 hours, room temperature

PRO F 639818-48-7

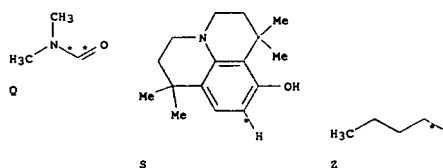
RX(2) RCT A 20205-30-5, F 639818-48-7  
RGT D 110-86-1 Pyridine  
PRO G 639818-44-3  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(47) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(2)  
AND REACTION SEQUENCE RX(7), RX(9), RX(2)  
...Z + AE ==> A...

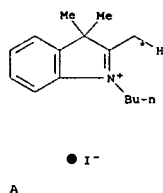
L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



START NEXT REACTION SEQUENCE



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
RGT D 110-86-1 Pyridine  
PRO A 20205-30-5  
SOL 78-93-3 EtOMe  
CON 6 hours, reflux

RX(7) RCT Q 68-12-2

STAGE(1)  
RGT W 10025-87-3 POCl3  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

RX(9) RCT V 115662-09-4

STAGE(1)  
RGT Y 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

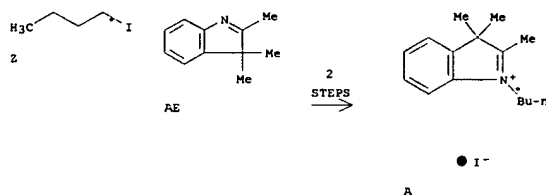
STAGE(2)  
RCT Z 542-69-8  
CON 12 hours, room temperature

PRO F 639818-48-7

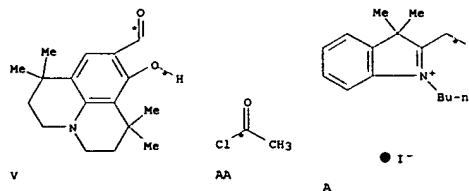
L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(2) RCT A 20205-30-5, F 639818-48-7  
RGT D 110-86-1 Pyridine  
PRO G 639818-44-3  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(48) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(3)  
AND REACTION SEQUENCE RX(10), RX(3)  
...Z + AE ==> A...  
...V + AA + A ==> I



START NEXT REACTION SEQUENCE

2  
STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

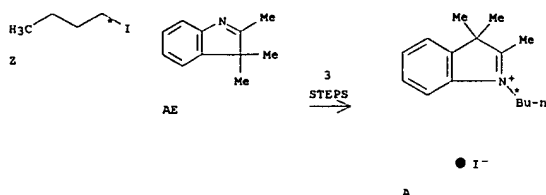
RX(12) RCT Z 542-69-8, AE 1640-39-7  
RGT D 110-86-1 Pyridine  
PRO A 20205-30-5  
SOL 78-93-3 EtOMe

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

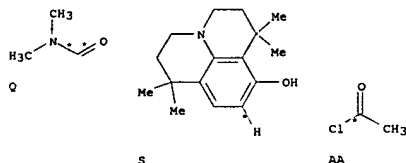
RX(10) RCT V 115662-09-4, AA 75-36-5  
RGT AB 121-44-8 Et3N  
PRO H 639818-49-8  
SOL 67-66-3 CHCl3  
CON 4 hours, room temperature

RX(3) RCT A 20205-30-5, H 639818-49-8  
RGT D 110-86-1 Pyridine  
PRO I 639818-45-4  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(49) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(3)  
AND REACTION SEQUENCE RX(7), RX(10), RX(3)  
...Z + AE ==> A...  
...Q + S + AA + A ==> I



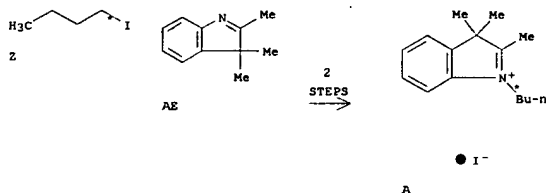
START NEXT REACTION SEQUENCE



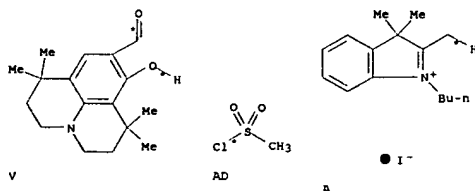
L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO I 639818-45-4  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(50) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(4)  
AND REACTION SEQUENCE RX(11), RX(4)  
...Z + AE ==> A...  
...V + AD + A ==> K



START NEXT REACTION SEQUENCE

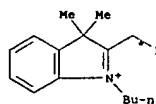


2  
STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
RGT D 110-86-1 Pyridine  
PRO A 20205-30-5  
SOL 78-93-3 EtCOMe  
CON 6 hours, reflux

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



• I<sup>-</sup>  
A  
3  
STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
RGT D 110-86-1 Pyridine  
PRO A 20205-30-5  
SOL 78-93-3 EtCOMe  
CON 6 hours, reflux

RX(7) RCT Q 68-12-2  
STAGE(1)  
RGT W 10025-87-3 POC13  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C  
STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

RX(10) RCT V 115662-09-4, AA 75-36-5  
RGT AB 121-44-8 Et3N  
PRO H 639818-49-8  
SOL 67-66-3 CHCl3  
CON 4 hours, room temperature

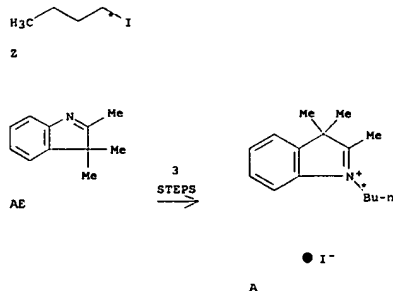
RX(3) RCT A 20205-30-5, H 639818-49-8  
RGT D 110-86-1 Pyridine

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

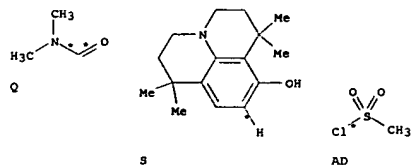
RX(11) RCT V 115662-09-4, AD 124-63-0  
RGT AB 121-44-8 Et3N  
PRO J 639818-50-1  
SOL 67-66-3 CHCl3  
CON 4 hours, room temperature

RX(4) RCT A 20205-30-5, J 639818-50-1  
RGT D 110-86-1 Pyridine  
PRO K 639818-46-5  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

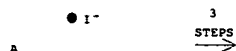
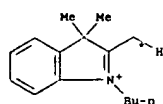
RX(51) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(4)  
AND REACTION SEQUENCE RX(7), RX(11), RX(4)  
...Z + AE ==> A...  
...Q + S + AD + A ==> K



START NEXT REACTION SEQUENCE



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
 RGT D 110-86-1 Pyridine  
 PRO A 20205-30-5  
 SOL 78-93-3 EtCOME  
 CON 6 hours, reflux

RX(7) RCT Q 68-12-2

STAGE(1)  
 RGT W 10025-87-3 POC13  
 SOL 68-12-2 DMF  
 CON 2 hours, 0 deg C

STAGE(2)  
 RCT S 115704-83-1  
 SOL 68-12-2 DMF  
 CON 12 hours, room temperature

STAGE(3)  
 RGT O 127-09-3 AcONa  
 SOL 7732-18-5 Water  
 CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
 NTE Vilsmeier-Haak reaction

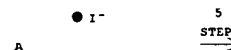
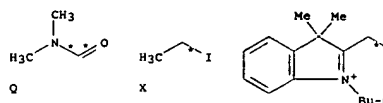
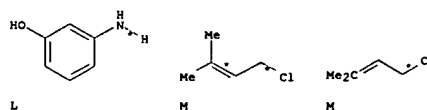
RX(11) RCT V 115662-09-4, AD 124-63-0  
 RGT AB 121-44-8 Et3N  
 PRO J 639818-50-1  
 SOL 67-66-3 CHCl3  
 CON 4 hours, room temperature

RX(4) RCT A 20205-30-5, J 639818-50-1  
 RGT D 110-86-1 Pyridine  
 PRO K 639818-46-5

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

RX(52) OF 63 COMPOSED OF RX(5), RX(6), RX(7), RX(8), RX(1)  
 RX(52) L + 2 M + Q + X + A ==> C



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT L 591-27-5, M 503-60-6

STAGE(1)  
 RGT O 127-09-3 AcONa  
 SOL 68-12-2 DMF  
 CON 12 hours, 30 deg C

STAGE(2)  
 RGT P 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON 0 deg C

PRO N 115662-07-2

RX(6) RCT N 115662-07-2

STAGE(1)  
 RGT T 75-75-2 MeSO3H

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

CON 2 hours, 95 deg C

STAGE(2)  
 RGT U 1336-21-6 NH4OH  
 SOL 7732-18-5 Water  
 CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

STAGE(1)  
 RGT W 10025-87-3 POC13  
 SOL 68-12-2 DMF  
 CON 2 hours, 0 deg C

STAGE(2)  
 RCT S 115704-83-1  
 SOL 68-12-2 DMF  
 CON 12 hours, room temperature

STAGE(3)  
 RGT O 127-09-3 AcONa  
 SOL 7732-18-5 Water  
 CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
 NTE Vilsmeier-Haak reaction

RX(8) RCT V 115662-09-4

STAGE(1)  
 RGT Y 7646-69-7 NaH  
 SOL 68-12-2 DMF  
 CON 2 hours, room temperature

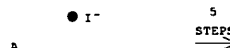
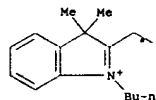
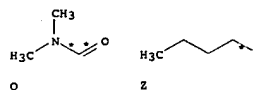
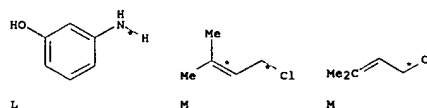
STAGE(2)  
 RCT X 75-03-6  
 CON 12 hours, room temperature

PRO B 639818-47-6

RX(1) RCT A 20205-30-5, B 639818-47-6  
 RGT D 110-86-1 Pyridine  
 PRO C 639818-43-2  
 SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

RX(53) OF 63 COMPOSED OF RX(5), RX(6), RX(7), RX(9), RX(2)  
 RX(53) L + 2 M + Q + Z + A ==> G

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT L 591-27-5, M 503-60-6

STAGE(1)  
 RGT O 127-09-3 AcONa  
 SOL 68-12-2 DMF  
 CON 12 hours, 30 deg C

STAGE(2)  
 RGT P 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON 0 deg C

PRO N 115662-07-2

RX(6) RCT N 115662-07-2

STAGE(1)  
 RGT T 75-75-2 MeSO3H  
 CON 2 hours, 95 deg C

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(2)  
RGT U 1336-21-6 NH4OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

STAGE(1)  
RGT W 10025-87-3 POC13  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

RX(9) RCT V 115662-09-4

STAGE(1)  
RGT Y 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

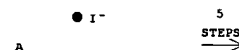
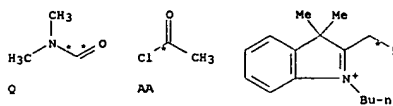
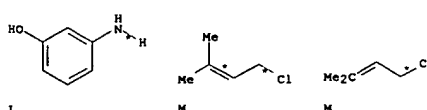
STAGE(2)  
RCT Z 542-69-8  
CON 12 hours, room temperature

PRO F 639818-48-7

RX(2) RCT A 20205-30-5, F 639818-48-7  
RGT D 110-86-1 Pyridine  
PRO G 639818-44-3  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(54) OF 63 COMPOSED OF RX(5), RX(6), RX(7), RX(10), RX(3)  
RX(54) L + 2 M + Q + AA + A ==> I

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT L 591-27-5, M 503-60-6

STAGE(1)  
RGT O 127-09-3 AcONa  
SOL 68-12-2 DMF  
CON 12 hours, 30 deg C

STAGE(2)  
RGT P 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 0 deg C

PRO N 115662-07-2

RX(6) RCT N 115662-07-2

STAGE(1)  
RGT T 75-75-2 MeSO3H  
CON 2 hours, 95 deg C

STAGE(2)  
RGT U 1336-21-6 NH4OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

STAGE(1)  
RGT W 10025-87-3 POC13  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

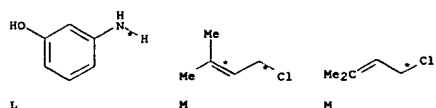
STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

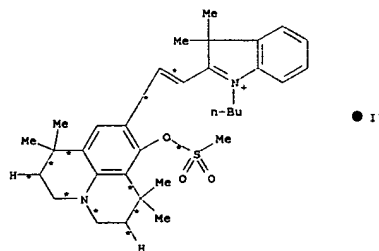
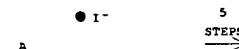
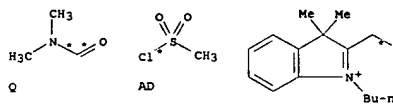
RX(10) RCT V 115662-09-4, AA 75-36-5  
RGT AB 121-44-8 Et3N  
PRO H 639818-49-8  
SOL 67-66-3 CHCl3  
CON 4 hours, room temperature

RX(3) RCT A 20205-30-5, H 639818-49-8  
RGT D 110-86-1 Pyridine  
PRO I 639818-45-4  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(55) OF 63 COMPOSED OF RX(5), RX(6), RX(7), RX(11), RX(4)  
RX(55) L + 2 M + Q + AD + A ==> K



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



K  
YIELD 74%

RX(5) RCT L 591-27-5, M 503-60-6

STAGE(1)  
RGT O 127-09-3 AcONa  
SOL 68-12-2 DMF  
CON 12 hours, 30 deg C

STAGE(2)  
RGT P 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 0 deg C

PRO N 115662-07-2

RX(6) RCT N 115662-07-2

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

## STAGE(1)

RGT T 75-75-2 MeSO<sub>3</sub>H  
CON 2 hours, 95 deg C

## STAGE(2)

RGT U 1336-21-6 NH<sub>4</sub>OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

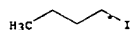
## STAGE(1)

RGT W 10025-87-3 POCl<sub>3</sub>  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

## STAGE(2)

RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

## STAGE(3)

RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8PRO V 115662-09-4  
NTE Vilsmeier-Haak reactionRX(11) RCT V 115662-09-4, AD 124-63-0  
RGT AB 121-44-8 Et<sub>3</sub>N  
PRO J 639818-50-1  
SOL 67-66-3 CHCl<sub>3</sub>  
CON 4 hours, room temperatureRX(4) RCT A 20205-30-5, J 639818-50-1  
RGT D 110-86-1 Pyridine  
PRO K 639818-46-5  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, refluxRX(56) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(1)  
AND REACTION SEQUENCE RX(6), RX(7), RX(8), RX(1)  
...Z + AE ==> A...  
...N + Q + X + A ==> C

Z

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
RGT D 110-86-1 Pyridine  
PRO A 20205-30-5  
SOL 78-93-3 EtCOMe  
CON 6 hours, reflux

RX(6) RCT N 115662-07-2

## STAGE(1)

RGT T 75-75-2 MeSO<sub>3</sub>H  
CON 2 hours, 95 deg C

## STAGE(2)

RGT U 1336-21-6 NH<sub>4</sub>OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

## STAGE(1)

RGT W 10025-87-3 POCl<sub>3</sub>  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

## STAGE(2)

RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

## STAGE(3)

RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

RX(8) RCT V 115662-09-4

## STAGE(1)

RGT Y 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

## STAGE(2)

RCT X 75-03-6  
CON 12 hours, room temperature

PRO B 639818-47-6

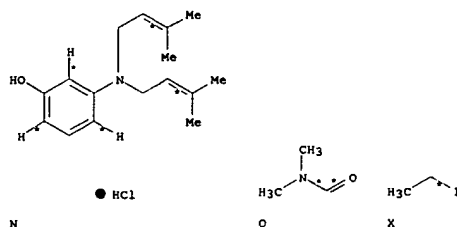
RX(11) RCT A 20205-30-5, B 639818-47-6  
RGT D 110-86-1 Pyridine  
PRO C 639818-43-2

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

• I<sup>-</sup>

A

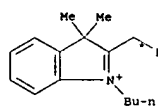
START NEXT REACTION SEQUENCE



N

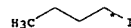
Q

X

• I<sup>-</sup>

A

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

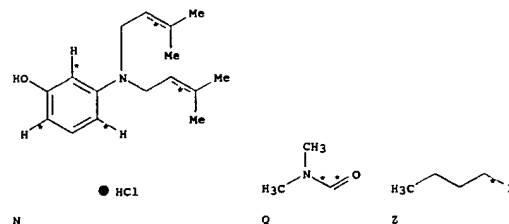
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, refluxRX(57) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(2)  
AND REACTION SEQUENCE RX(6), RX(7), RX(9), RX(2)  
...Z + AE ==> A...  
...N + Q + Z + A ==> G

Z

• I<sup>-</sup>

A

START NEXT REACTION SEQUENCE



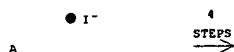
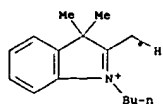
N

Q

Z



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
RGT D 110-86-1 Pyridine  
PRO A 20205-30-5  
SOL 78-93-3 EtCOMe  
CON 6 hours, reflux

RX(6) RCT N 115662-07-2

STAGE(1)  
RGT T 75-75-2 MeSO<sub>3</sub>H  
CON 2 hours, 95 deg C

STAGE(2)  
RGT U 1336-21-6 NH<sub>4</sub>OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

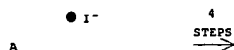
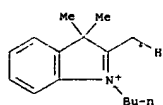
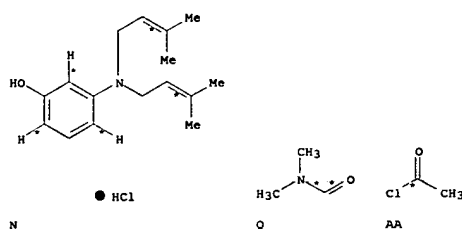
RX(7) RCT Q 68-12-2

STAGE(1)  
RGT W 10025-87-3 POCl<sub>3</sub>  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
RGT D 110-86-1 Pyridine  
PRO A 20205-30-5  
SOL 78-93-3 EtCOMe  
CON 6 hours, reflux

RX(6) RCT N 115662-07-2

STAGE(1)  
RGT T 75-75-2 MeSO<sub>3</sub>H  
CON 2 hours, 95 deg C

STAGE(2)  
RGT U 1336-21-6 NH<sub>4</sub>OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

RX(9) RCT V 115662-09-4

STAGE(1)  
RCT Y 7646-69-7 NaH  
SOL 68-12-2 DMF  
CON 2 hours, room temperature

STAGE(2)  
RCT Z 542-69-8  
CON 12 hours, room temperature

PRO F 639818-48-7

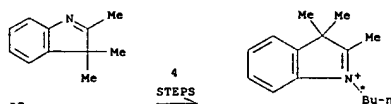
RX(2) RCT A 20205-30-5, F 639818-48-7  
RGT D 110-86-1 Pyridine  
PRO G 639818-44-3  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(58) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(3)  
AND REACTION SEQUENCE RX(6), RX(7), RX(10), RX(3)

...Z + AE ==> A...  
...N + Q + AA + A ==> I



Z



AE

● I<sup>-</sup>

A

START NEXT REACTION SEQUENCE

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(7) RCT Q 68-12-2

STAGE(1)  
RGT W 10025-87-3 POCl<sub>3</sub>  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)  
RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

STAGE(3)  
RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
NTE Vilsmeier-Haak reaction

RX(10) RCT V 115662-09-4, AA 75-36-5  
RGT AB 121-44-8 Et<sub>3</sub>N  
PRO H 639818-49-8  
SOL 67-66-3 CHCl<sub>3</sub>  
CON 4 hours, room temperature

RX(3) RCT A 20205-30-5, H 639818-49-8  
RGT D 110-86-1 Pyridine  
PRO I 639818-45-4  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

RX(59) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(4)  
AND REACTION SEQUENCE RX(6), RX(7), RX(11), RX(4)

...Z + AE ==> A...  
...N + Q + AD + A ==> K

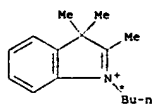


Z

AE

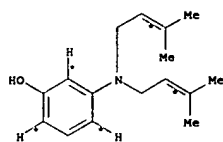
4  
STEPS

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● I<sup>-</sup>

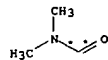
A

START NEXT REACTION SEQUENCE



● HCl

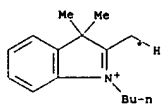
N



Q



AD

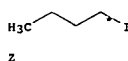
● I<sup>-</sup>

A

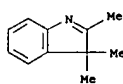
4  
STEPS

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

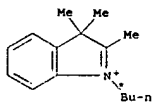
RX(60) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(1)  
AND REACTION SEQUENCE RX(5), RX(6), RX(7), RX(8), RX(1)  
...Z + AE ==> A...  
...L + 2 M + Q + X + A ==> C



Z

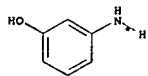


AE

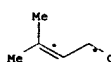
5  
STEPS● I<sup>-</sup>

A

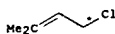
START NEXT REACTION SEQUENCE



L



M



M

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
RGT D 110-86-1 Pyridine  
PRO A 20205-30-5  
SOL 78-93-3 EtCOMe  
CON 6 hours, reflux

RX(6) RCT N 115662-07-2

STAGE(1)

RGT T 75-75-2 MeSO<sub>3</sub>H  
CON 2 hours, 95 deg C

STAGE(2)

RGT U 1336-21-6 NH<sub>4</sub>OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

STAGE(1)

RGT W 10025-87-3 POC13  
SOL 68-12-2 DMF  
CON 2 hours, 0 deg C

STAGE(2)

RCT S 115704-83-1  
SOL 68-12-2 DMF  
CON 12 hours, room temperature

STAGE(3)

RGT O 127-09-3 AcONa  
SOL 7732-18-5 Water  
CON overnight, 0 deg C, pH 7 - 8

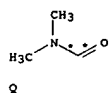
PRO V 115662-09-4

NTE Vilsmeier-Haak reaction

RX(11) RCT V 115662-09-4, AD 124-63-0  
RGT AB 121-44-8 Et<sub>3</sub>N  
PRO J 639818-50-1  
SOL 67-66-3 CHCl<sub>3</sub>  
CON 4 hours, room temperature

RX(4) RCT A 20205-30-5, J 639818-50-1  
RGT D 110-86-1 Pyridine  
PRO K 639818-46-5  
SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
CON overnight, reflux

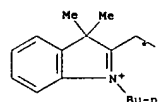
L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



Q



X

● I<sup>-</sup>

A

5  
STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
RGT D 110-86-1 Pyridine  
PRO A 20205-30-5  
SOL 78-93-3 EtCOMe  
CON 6 hours, reflux

RX(5) RCT L 591-27-5, M 503-60-6

STAGE(1)

RGT O 127-09-3 AcONa  
SOL 68-12-2 DMF  
CON 12 hours, 30 deg C

STAGE(2)

RGT P 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON 0 deg C

PRO N 115662-07-2

RX(6) RCT N 115662-07-2

STAGE(1)

RGT T 75-75-2 MeSO<sub>3</sub>H  
CON 2 hours, 95 deg C

STAGE(2)

RGT U 1336-21-6 NH<sub>4</sub>OH  
SOL 7732-18-5 Water  
CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

STAGE(1)

RGT W 10025-87-3 POC13  
SOL 68-12-2 DMF



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
 RGT D 110-86-1 Pyridine  
 PRO A 20205-30-5  
 SOL 78-93-3 EtCOMe  
 CON 6 hours, reflux

RX(5) RCT L 591-27-5, M 503-60-6

STAGE(1)  
 RGT O 127-09-3 AcONa  
 SOL 68-12-2 DMF  
 CON 12 hours, 30 deg C

STAGE(2)  
 RGT P 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON 0 deg C

PRO N 115662-07-2

RX(6) RCT N 115662-07-2

STAGE(1)  
 RGT T 75-75-2 MeSO3H  
 CON 2 hours, 95 deg C

STAGE(2)  
 RGT U 1336-21-6 NH4OH  
 SOL 7732-18-5 Water  
 CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

STAGE(1)  
 RGT W 10025-87-3 POCl3  
 SOL 68-12-2 DMF  
 CON 2 hours, 0 deg C

STAGE(2)  
 RCT S 115704-83-1  
 SOL 68-12-2 DMF  
 CON 12 hours, room temperature

STAGE(3)  
 RGT O 127-09-3 AcONa  
 SOL 7732-18-5 Water  
 CON overnight, 0 deg C, pH 7 - 8

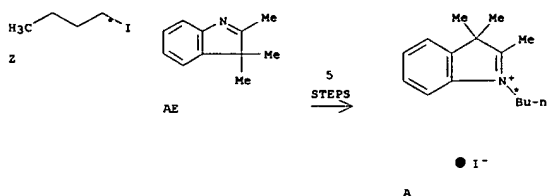
PRO V 115662-09-4

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

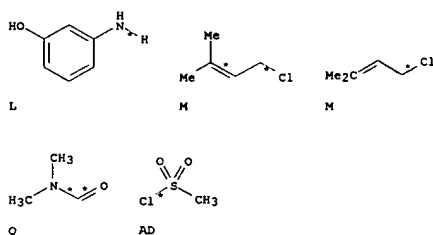
RX(10) RCT V 115662-09-4, AA 75-36-5  
 RGT AB 121-44-8 Et3N  
 PRO H 639818-49-8  
 SOL 67-66-3 CHCl3  
 CON 4 hours, room temperature

RX(3) RCT A 20205-30-5, H 639818-49-8  
 RGT D 110-86-1 Pyridine  
 PRO I 639818-45-4  
 SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

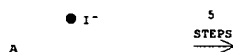
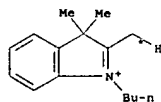
RX(63) OF 63 COMPOSED OF REACTION SEQUENCE RX(12), RX(4)  
 AND REACTION SEQUENCE RX(5), RX(6), RX(7), RX(11), RX(4)  
 ...Z + AE ==> A...  
 ...L + 2 M + Q + AD + A ==> K



START NEXT REACTION SEQUENCE



L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(12) RCT Z 542-69-8, AE 1640-39-7  
 RGT D 110-86-1 Pyridine  
 PRO A 20205-30-5  
 SOL 78-93-3 EtCOMe  
 CON 6 hours, reflux

RX(5) RCT L 591-27-5, M 503-60-6

STAGE(1)  
 RGT O 127-09-3 AcONa  
 SOL 68-12-2 DMF  
 CON 12 hours, 30 deg C

STAGE(2)  
 RGT P 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON 0 deg C

PRO N 115662-07-2

RX(6) RCT N 115662-07-2

STAGE(1)  
 RGT T 75-75-2 MeSO3H  
 CON 2 hours, 95 deg C

STAGE(2)  
 RGT U 1336-21-6 NH4OH  
 SOL 7732-18-5 Water  
 CON 0 deg C, pH 7 - 8

PRO S 115704-83-1

RX(7) RCT Q 68-12-2

STAGE(1)  
 RGT W 10025-87-3 POCl3

L2 ANSWER 15 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 68-12-2 DMF  
 CON 2 hours, 0 deg C

STAGE(2)  
 RCT S 115704-83-1  
 SOL 68-12-2 DMF  
 CON 12 hours, room temperature

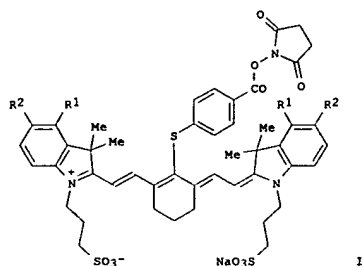
STAGE(3)  
 RGT O 127-09-3 AcONa  
 SOL 7732-18-5 Water  
 CON overnight, 0 deg C, pH 7 - 8

PRO V 115662-09-4  
 NTE Vilsmeier-Haak reaction

RX(11) RCT V 115662-09-4, AD 124-63-0  
 RGT AB 121-44-8 Et3N  
 PRO J 639818-50-1  
 SOL 67-66-3 CHCl3  
 CON 4 hours, room temperature

RX(4) RCT A 20205-30-5, J 639818-50-1  
 RGT D 110-86-1 Pyridine  
 PRO K 639818-46-5  
 SOL 1320-67-8 Propanol, 1(or 2)-methoxy-  
 CON overnight, reflux

L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 14078500 CASREACT  
 TITLE: Synthesis of water-soluble near-infrared cyanine dyes  
 functionalized with ((succinimido)oxyl)carbonyl group  
 AUTHOR(S): Strekowski, Lucjan; Mason, Christian J.; Lee, Myeran;  
 Gupta, Rajni; Sowell, John; Patonay, Gabor  
 CORPORATE SOURCE: Department of Chemistry, Georgia State University,  
 Atlanta, GA, 30303, USA  
 SOURCE: Journal of Heterocyclic Chemistry (2003), 40(5),  
 913-916  
 CODEN: JHCTAD; ISSN: 0022-152X  
 PUBLISHER: HeteroCorporation  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

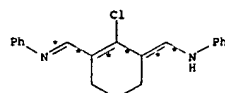
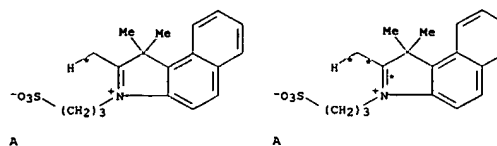


AB Two heptamethine cyanine dyes I [R1 = R2 = H; R1R2 = (CH:CH)2] suitable for labeling of biomols. at a primary amino group with a near-IR chromophore/fluorophore ( $\lambda_{max}/\lambda_{em}$  = 800/830 nm and 837/864 nm) have been synthesized from readily available starting materials. Despite the high mol. complexity of intermediate and final products, all these compds. have been obtained in an anal. pure form by using crystallization only.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

RX(1) OF 13 ...2 A + B ==> C...

L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● HCl

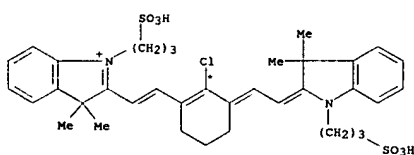
(1) →

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 63666-10-4, B 63857-00-1  
 RGT D 127-09-3 AcONa  
 PRO C 640279-12-5  
 SOL 64-17-5 EtOH  
 NTE stereoselective

RX(2) OF 13 F + G ==> H...

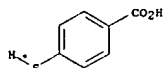
L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



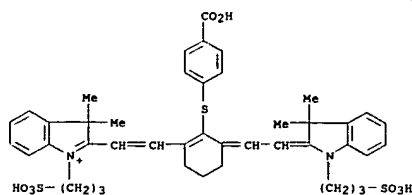
● Cl<sup>-</sup>

● 2 Na

F



(2) →



● Cl<sup>-</sup>

PAGE 1-A

L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

● 2 Na

H  
 YIELD 66%

RX(2) RCT F 537040-07-6, G 1074-36-8

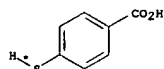
STAGE(1)  
 SOL 68-12-2 DMF  
 CON 24 hours, 23 deg C

STAGE(2)  
 SOL 64-17-5 EtOH, 60-29-7 Et2O

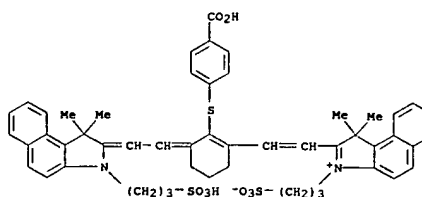
PRO H 537040-09-8

RX(3) OF 13 ...C + G ==> K...

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



(3) →



● Na

K  
 YIELD 90%

L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

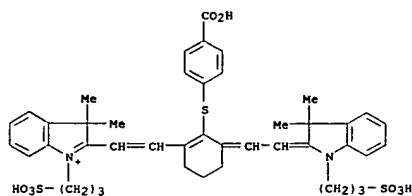
RX(3) RCT C 640279-12-5, G 1074-36-8

STAGE(1)  
 SOL 68-12-2 DMF  
 CON 24 hours, 23 deg C

STAGE(2)  
 SOL 64-17-5 EtOH, 60-29-7 Et2O

PRO K 367251-79-4

RX(4) OF 13 ...H + L ==&gt; M

● Cl<sup>-</sup>

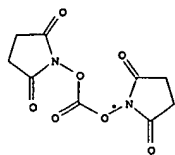
● 2 Na

H

PAGE 1-A

PAGE 2-A

L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L (4) →

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A

● Cl<sup>-</sup>

● 2 Na

M  
YIELD 90%

RX(4) RCT H 537040-09-8, L 74124-79-1

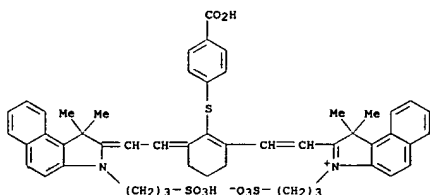
STAGE(1)  
 SOL 68-12-2 DMF  
 CON 24 hours, 23 deg C

STAGE(2)  
 SOL 60-29-7 Et2O  
 CON 30 minutes, 23 deg C

PRO M 640279-13-6

RX(5) OF 13 ...K + L ==&gt; N

L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

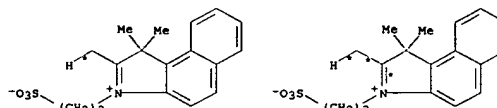
K

L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 60-29-7 Et2O  
 CON 30 minutes, 23 deg C

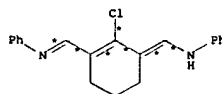
PRO N 367251-80-7

RX(7) OF 13 COMPOSED OF RX(1), RX(3)  
 RX(7) 2 A + B + G ==> K



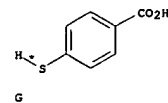
A

A



● HCl

B



G

2  
STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A

● Na

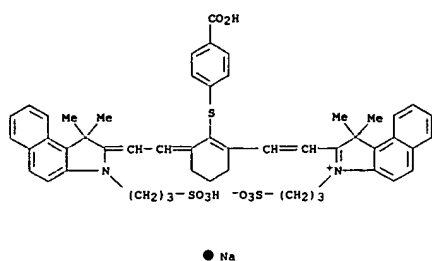
N  
YIELD 88%

RX(5) RCT K 367251-79-4, L 74124-79-1

STAGE(1)  
 SOL 68-12-2 DMF  
 CON 24 hours, 23 deg C

STAGE(2)

L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

K  
YIELD 90%

RX(1) RCT A 63666-10-4, B 63857-00-1  
RGT D 127-09-3 AcONa  
PRO C 640279-12-5  
SOL 64-17-5 EtOH  
NTE stereoselective

RX(3) RCT C 640279-12-5, G 1074-36-8

STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, 23 deg C

STAGE(2)  
SOL 64-17-5 EtOH, 60-29-7 Et2O

PRO K 367251-79-4

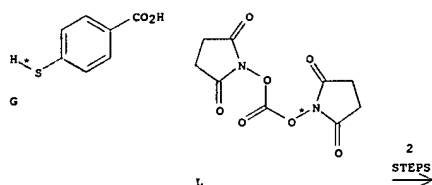
RX(8) OF 13 COMPOSED OF RX(2), RX(4)  
RX(8) F + G + L ==> M

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
PRO M 640279-13-6

RX(9) OF 13 COMPOSED OF RX(3), RX(5)  
RX(9) C + G + L ==> N

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A

N  
YIELD 88%

RX(3) RCT C 640279-12-5, G 1074-36-8

STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, 23 deg C

STAGE(2)  
SOL 64-17-5 EtOH, 60-29-7 Et2O

PRO K 367251-79-4

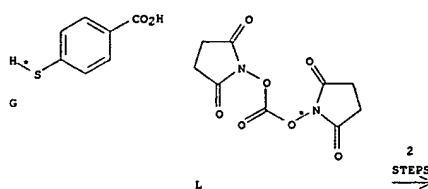
RX(5) RCT K 367251-79-4, L 74124-79-1

STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, 23 deg C

STAGE(2)  
SOL 60-29-7 Et2O  
CON 30 minutes, 23 deg C

PRO N 367251-80-7

L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A

M  
YIELD 90%

RX(2) RCT F 537040-07-6, G 1074-36-8

STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, 23 deg C

STAGE(2)  
SOL 64-17-5 EtOH, 60-29-7 Et2O

PRO H 537040-09-8

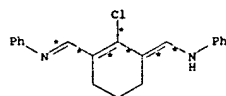
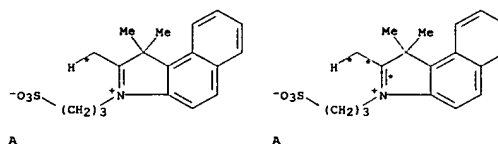
RX(4) RCT H 537040-09-8, L 74124-79-1

STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, 23 deg C

STAGE(2)  
SOL 60-29-7 Et2O  
CON 30 minutes, 23 deg C

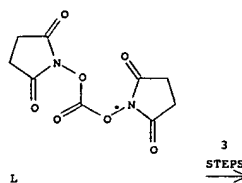
L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(11) OF 13 COMPOSED OF RX(1), RX(3), RX(5)  
RX(11) 2 A + B + G + L ==> N



B

G



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

L2 ANSWER 16 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

● Na

N  
YIELD 88%

RX(1) RCT A 63666-10-4, B 63857-00-1  
RGT D 127-09-3 AcONa  
PRO C 640279-12-5  
SOL 64-17-5 EtOH  
NTE stereoselective

RX(3) RCT C 640279-12-5, G 1074-36-8

STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, 23 deg C

STAGE(2)  
SOL 64-17-5 EtOH, 60-29-7 Et2O

PRO K 367251-79-4

RX(5) RCT K 367251-79-4, L 74124-79-1

STAGE(1)  
SOL 68-12-2 DMF  
CON 24 hours, 23 deg C

STAGE(2)  
SOL 60-29-7 Et2O  
CON 30 minutes, 23 deg C

PRO N 367251-80-7

L2 ANSWER 17 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

139:366344 CASREACT

TITLE:

Hemicyanine n-butyltriphenylborate salts as effective  
initiators of free-radical polymerization  
photoinitiated via photoinduced electron-transfer  
process

AUTHOR(S):

Kabato, Janina; Jedrzejewska, Beata; Paczkowski,

CORPORATE SOURCE:

Faculty of Chemical Technology and Engineering,  
University of Technology and Agriculture, Bydgoszcz,  
85-326, Pol.

SOURCE:

Journal of Polymer Science, Part A: Polymer Chemistry  
(2003), 41(19), 3017-3026  
CODEN: JPACEC; ISSN: 0887-624X

PUBLISHER:

John Wiley &amp; Sons, Inc.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB

Two different groups of hemicyanine BuBPh3- salts (HCBs) were synthesized and examined to verify the possibility of applying the Marcus equation to the description of the kinetics of free-radical polymerization of trimethylolpropane triacrylate photoinitiated via the photoinduced electron-transfer process. The free-energy change ( $\Delta G$ ) of the electron-transfer process between an excited acceptor and a donor were exptl. determined for 14 new organic photoredox pairs. The relationship between

the rate of polymerization and the free-energy change for the electron-transfer

process displayed typical Marcus kinetic behavior. The photoredn. of the HCBs produced colorless products. The exptl. results indicated that the rate of the light-absorber bleaching process does not compete with the photoinitiation of polymerization

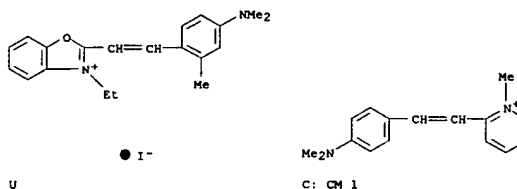
REFERENCE COUNT:

25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS

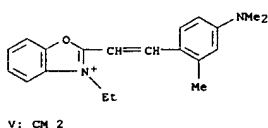
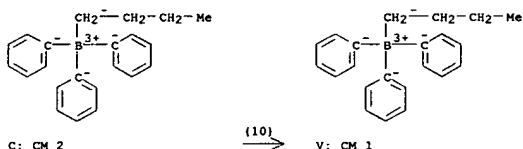
FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(10) OF 20 ...U + C ==&gt; V

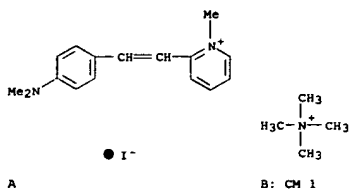


L2 ANSWER 17 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

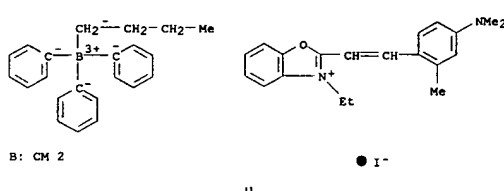
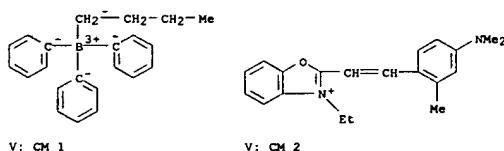


RX(10) RCT U 612839-70-0, C 620551-94-2  
PRO V 620552-13-8  
SOL 75-05-8 MeCN  
NTE no exptl. detail

RX(16) OF 20 COMPOSED OF RX(1), RX(10)  
RX(16) A + B + U ==> V



L2 ANSWER 17 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

2  
STEPS

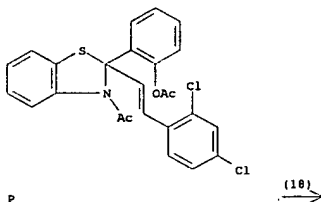
RX(1) RCT A 2156-29-8, B 117522-01-7  
PRO C 620551-94-2  
SOL 75-05-8 MeCN  
NTE no exptl. detail

RX(10) RCT U 612839-70-0, C 620551-94-2  
PRO V 620552-13-8  
SOL 75-05-8 MeCN  
NTE no exptl. detail

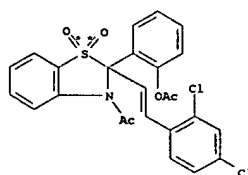


L2 ANSWER 18 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 139:350659 CASREACT  
 TITLE: Chemoselective oxidation of 3-acetyl-2,3-dihydrobenzothiazoles by dimethyldioxirane  
 AUTHOR(S): Levai, Albert; Jeko, Jozsef  
 CORPORATE SOURCE: Department of Organic Chemistry, University of Debrecen, Debrecen, H-4010, Hung.  
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2003), (5), 19-27  
 CODEN: AGPUAR  
 URL: <http://www.arkat-usa.org/ark/journal/2003/Bernath/GB-642J/642J.pdf>  
 PUBLISHER: Arkat USA Inc.  
 DOCUMENT TYPE: Journal; (online computer file)  
 LANGUAGE: English  
 AB 3-Acetyl-2,3-dihydrobenzothiazole derivs. (I) were prepared by the ring contraction of 2,4-diaryl-2,3-dihydro-1,5-benzothiazepines under acetylating conditions. Some of the I were oxidized with dimethyldioxirane in acetone solution at ambient temperature to afford 3-acetyl-2,3-dihydrobenzothiazole 1,1-dioxides as sole products.  
 REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS  
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(18) OF 28 ...P ==> AK



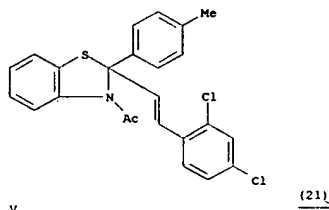
L2 ANSWER 18 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



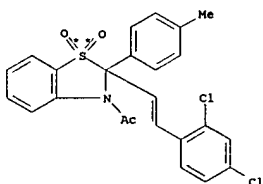
AK  
 YIELD 78%

RX(18) RCT P 618114-03-7  
 RGT Y 74087-85-7 Dimethyldioxirane  
 PRO AK 618114-15-1  
 SOL 75-09-2 CH2Cl2, 67-64-1 Me2CO  
 CON 16 hours, room temperature  
 NTE chemoselective

RX(21) OF 28 ...V ==> AN



L2 ANSWER 18 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

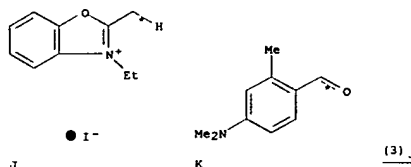


AN  
 YIELD 78%

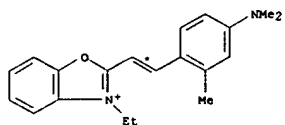
RX(21) RCT V 618114-06-0  
 RGT Y 74087-85-7 Dimethyldioxirane  
 PRO AN 618114-18-4  
 SOL 75-09-2 CH2Cl2, 67-64-1 Me2CO  
 CON 16 hours, room temperature  
 NTE chemoselective

L2 ANSWER 19 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 139:324741 CASREACT  
 TITLE: Hemicyanine dyes: synthesis, structure and photophysical properties  
 AUTHOR(S): Jedrzejewska, Beata; Kabatc, Janina; Pietrzak, Marek; Paczkowski, Jerzy  
 CORPORATE SOURCE: Faculty of Chemical Technology and Engineering, University of Technology and Agriculture, Bydgoszcz, 85-326, Pol.  
 SOURCE: Dyes and Pigments (2003), 58(1), 47-58  
 CODEN: DYPIDX; ISSN: 0143-7208  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Cationic hemicyanine dyes such as 3-ethyl-2-[4-(diethylamino)styryl]benzoxazolium salts, 2-[4-(diethylamino)styryl]-1-(4-iodobenzyl)pyridinium salts, and 2-[4-(diethylamino)styryl]-1-methyl-6-iodopyridinium salts were synthesized and characterized. The dyes were prepared by the condensation of 3-ethyl-2-methylbenzoxazole salts, 1-(4-iodobenzyl)-2-methylpyridinium salts, or 1,2-dimethyl-6-iodopyridinium salts with p-(diethylamino)benzaldehydes. Three groups of chromophores with the same acceptor group but with various donor groups were obtained. The spectroscopic properties of the prepared dyes were determined in organic solvents.  
 REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS  
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(3) OF 48 ...J + K ==> L



L2 ANSWER 19 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

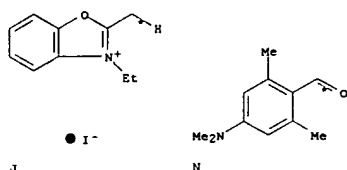
● I<sup>-</sup>L  
YIELD 26%

RX(3) RCT J 5260-37-7, K 1199-59-3

STAGE(1)  
SOL 108-24-7 Ac2O  
CON 20 minutes, refluxSTAGE(2)  
RGT D 7681-11-0 KI  
SOL 67-56-1 MeOH

PRO L 612839-70-0

RX(4) OF 48 ...J + N ==&gt; O

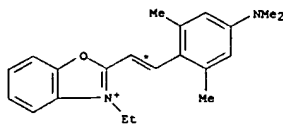
● I<sup>-</sup>

J

N

(4) →

L2 ANSWER 19 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● I<sup>-</sup>O  
YIELD 24%

RX(4) RCT J 5260-37-7, N 4980-19-2

STAGE(1)  
SOL 108-24-7 Ac2O  
CON 20 minutes, refluxSTAGE(2)  
RGT D 7681-11-0 KI  
SOL 67-56-1 MeOH

PRO O 612839-71-1

X

L2 ANSWER 20 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

TITLE:

139:262235 CASREACT  
Metallochromic merocyanines of 8-hydroxyquinoline series  
Kovtun, Yu. P.; Prostota, Ya. O.; Tolmachev, A. I.  
Institute of Organic Chemistry, National Academy of Sciences of Ukraine, Kiev, 03660, Ukraine  
Dyes and Pigments (2003), 58(1), 83-91  
CODEN: DYPIDX; ISSN: 0143-7208

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

AB A number of merocyanines based on the 5- and 7-substituted 8-hydroxyquinoline

nucleus have been synthesized, and the metallochromic and some metallofluorochromic properties of the prepared dyes have been studied.

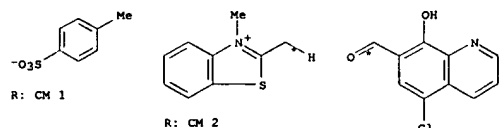
The most pronounced metallochromic effects are observed for dyes containing low-basicity end nuclei. Maximum metallofluorochromic effects were demonstrated by the 7-substituted derivs. of 8-hydroxyquinoline upon interaction with Zn<sup>2+</sup>, Cd<sup>2+</sup>, and Hg<sup>2+</sup> cations. A possible mechanism of metal binding is discussed.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

RX(7) OF 10 R + H ==&gt; B...

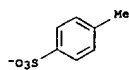


R: CM 1

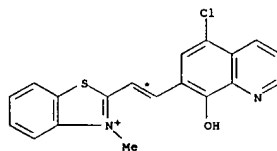
R: CM 2

H

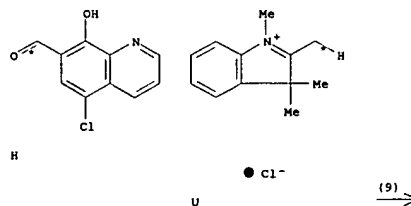
(7) →

S: CM 1  
YIELD 63%

L2 ANSWER 20 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

S: CM 2  
YIELD 63%RX(7) RCT R 2654-52-6, H 90876-69-0  
PRO S 603065-68-5  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

RX(9) OF 10 H + U ==&gt; V

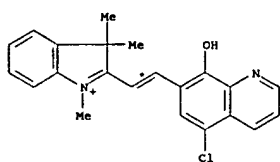
● Cl<sup>-</sup>

U

(9) →

X

L2 ANSWER 20 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

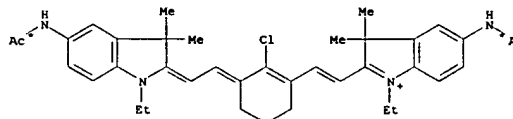
● Cl<sup>-</sup>V  
YIELD 70%

RX(9) RCT H 90876-69-0, U 62439-66-1  
PRO V 603065-70-9  
SOL 64-17-5 EtOH  
CON 5 hours, reflux

L2 ANSWER 21 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 139:70439 CASREACT  
TITLE: Boron trifluoride-methanol complex-mild and powerful reagent for deprotection of labile acetylated amines  
AUTHOR(S): Miltsov, Serguei; Rivera, Laia; Encinas, Cristina; Alonso, Julian  
CORPORATE SOURCE: Facultat de Ciències, Unitat de Química Analítica, Grup de Sensors i Biosensors, Universitat Autònoma de Barcelona, Bellaterra, 08193, Spain  
SOURCE: Tetrahedron Letters (2003), 44(11), 2301-2303  
CODEN: TELEAY; ISSN: 0040-4039  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A set of amino-group possessing cyanine dyes is obtained from their N-acetyl derivs. via deprotection with boron trifluoride-methanol complex in good yields.  
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

RX(1) OF 6 A ==&gt; B

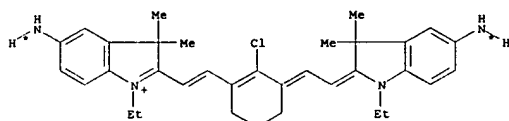
● I<sup>-</sup>

A

(1) →

X

L2 ANSWER 21 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● I<sup>-</sup>B  
YIELD 95%

RX(1) RCT A 548491-82-3  
RGT C 373-57-9 BF3.MeOH  
PRO B 548491-89-0  
SOL 67-56-1 MeOH  
CON reflux

RX(3) OF 6 G ==&gt; H

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

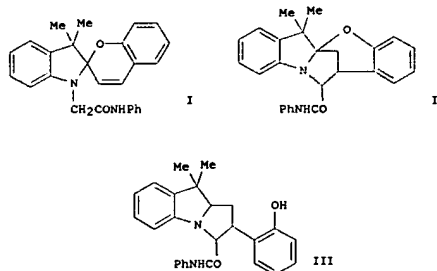
(3) →

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(3) RCT G 548491-83-4  
RGT C 373-57-9 BF3.MeOH  
PRO H 548491-91-4  
SOL 67-56-1 MeOH  
CON reflux

L2 ANSWER 22 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 138:401560 CASREACT  
TITLE: Rearrangement of spiro[2H-1-benzopyran-2,2'-(2H)indoles] to pyrrolo[1,2-a]indole derivatives  
AUTHOR(S): Martynaitis, Vytas; Sackus, Algirdas; Berg, Ulf  
CORPORATE SOURCE: Department of Organic Chemistry, Kaunas University of Technology, Kaunas, LT-3028, Lithuania  
SOURCE: Journal of Heterocyclic Chemistry (2002), 39(6), 1123-1128  
CODEN: JHTCAD; ISSN: 0022-152X  
PUBLISHER: HeteroCorporation  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

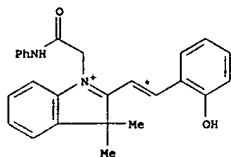
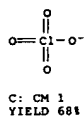
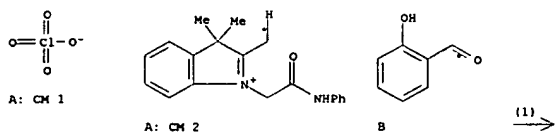


AB Heating of 1'-(N-substituted carbamoyl)methylspiro[2H-1-benzopyran-2,2'-(2H)indoles], e.g., I, with potassium hydroxide in ethanol yields diastereomeric 5a,13-methano-6H-1,3-benzoxazepino[3,2-a]indole-12-carboxamides, e.g., II. Reduction of the latter with sodium borohydride affords 1,2,3,9a-tetrahydro-2-(hydroxyaryl)-9H-pyrrolo[1,2-a]indole-3-carboxamides, e.g., III.

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

RX(1) OF 57 ...A + B ==&gt; C...

L2 ANSWER 22 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



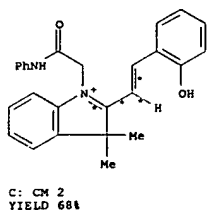
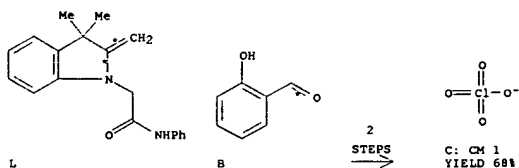
RX(1) RCT A 528839-64-7, B 90-02-8  
 STAGE(1)  
 RGT D 110-89-4 Piperidine  
 SOL 64-17-5 EtOH  
 CON 3 hours, reflux  
 STAGE(2)  
 RGT E 127-09-3 AcONa  
 STAGE(3)  
 SOL 60-29-7 Et2O  
 STAGE(4)

L2 ANSWER 22 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 64-17-5 EtOH  
 CON 3 hours, reflux  
 STAGE(2)  
 RGT E 127-09-3 AcONa  
 STAGE(3)  
 SOL 60-29-7 Et2O  
 STAGE(4)  
 RGT F 7601-90-3 HClO4  
 SOL 64-17-5 EtOH  
 CON 12 hours, 0 deg C, pH 2

PRO N 528839-68-1  
 NTE stereoselective

RX(21) OF 57 COMPOSED OF RX(3), RX(1)  
 RX(21) L + B ==> C



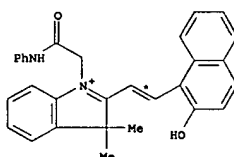
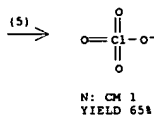
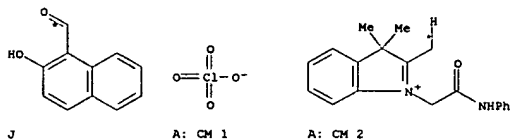
RX(3) RCT L 110789-60-1  
 RGT F 7601-90-3 HClO4  
 PRO A 528839-64-7  
 SOL 64-17-5 EtOH

L2 ANSWER 22 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RGT F 7601-90-3 HClO4  
 SOL 64-17-5 EtOH  
 CON 12 hours, 0 deg C, pH 2

PRO C 528839-66-9  
 NTE stereoselective

RX(5) OF 57 ...J + A ==> N...



RX(5) RCT J 708-06-5, A 528839-64-7  
 STAGE(1)  
 RGT D 110-89-4 Piperidine

L2 ANSWER 22 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

CON 12 hours, -5 deg C, pH 2

RX(1) RCT A 528839-64-7, B 90-02-8

STAGE(1)  
 RGT D 110-89-4 Piperidine  
 SOL 64-17-5 EtOH  
 CON 3 hours, reflux

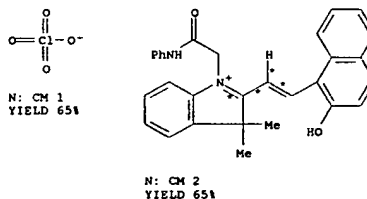
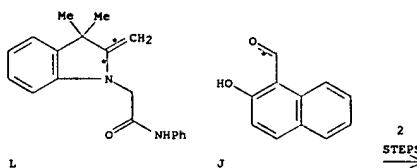
STAGE(2)  
 RGT E 127-09-3 AcONa

STAGE(3)  
 SOL 60-29-7 Et2O

STAGE(4)  
 RGT F 7601-90-3 HClO4  
 SOL 64-17-5 EtOH  
 CON 12 hours, 0 deg C, pH 2

PRO C 528839-66-9  
 NTE stereoselective

RX(22) OF 57 COMPOSED OF RX(3), RX(5)  
 RX(22) L + J ==> N



L2 ANSWER 22 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(3) RCT L 110789-60-1  
 RGT F 7601-90-3 HClO4  
 PRO A 528839-64-7  
 SOL 64-17-5 EtOH  
 CON 12 hours, -5 deg C, pH 2

RX(5) RCT J 708-06-5, A 528839-64-7

STAGE(1)  
 RGT D 110-89-4 Piperidine  
 SOL 64-17-5 EtOH  
 CON 3 hours, reflux

STAGE(2)  
 RGT E 127-09-3 AcONa

STAGE(3)  
 SOL 60-29-7 Et2O

STAGE(4)  
 RGT F 7601-90-3 HClO4  
 SOL 64-17-5 EtOH  
 CON 12 hours, 0 deg C, pH 2

PRO N 528839-68-1  
 NTE stereoselective

L2 ANSWER 23 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 137:156099 CASREACT  
 TITLE: Some new symmetric rigidified triheterocyclic heptamethinecyanine dyes absorbing in the near infrared

AUTHOR(S): Ramos, S. S.; Santos, P. F.; Reis, L. V.; Almeida, P.  
 CORPORATE SOURCE: Departamento de Quimica e Unidade de I & D de Materiais Texteis e Papeleiros, Universidade da Beira Interior, Covilha, 6201-001, Port.

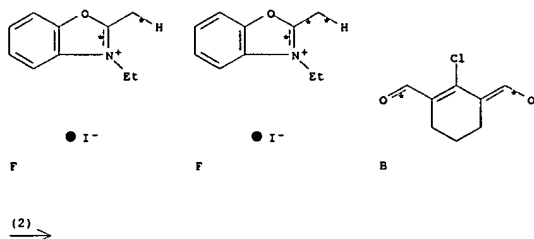
SOURCE: Dyes and Pigments (2002), 53(2), 143-152  
 CODEN: DYPIDX; ISSN: 0143-7208  
 PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal  
 LANGUAGE: English

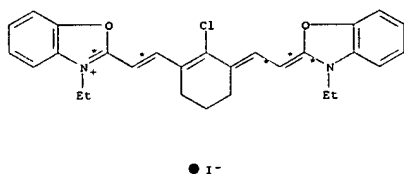
AB Several new rigidified heptamethine cyanine dyes bearing different N-alkyl chains were readily prepared by a novel semi-catalyzed method. All dyes displayed absorption within the so-called "phototherapeutic window". In order to improve the structural versatility of the dyes, a Cl atom was incorporated in the exocyclic conjugated bridge present in the polymethine chain. In some cases the Cl underwent an unexpected in-situ substitution by a third oxygenated heterocyclic group, depending on the solubility of the chloro dye in the reaction solvent. Two possible mechanisms for the formation of these triheterocyclic dyes are proposed. The full spectroscopic characterization of all the cyanines synthesized is described.

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

RX(2) OF 10 2 F + B ==&gt; G



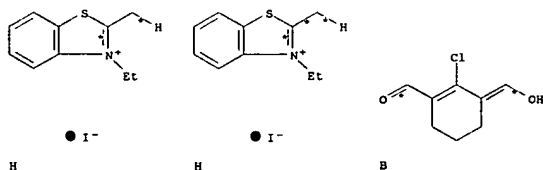
L2 ANSWER 23 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



G  
 YIELD 25%

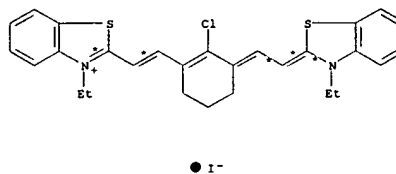
RX(2) RCT F 5260-37-7, B 61010-04-6  
 PRO G 162411-25-8  
 SOL 71-36-3 BuOH, 71-43-2 Benzene

RX(3) OF 10 2 H + B ==&gt; I...



(3) →

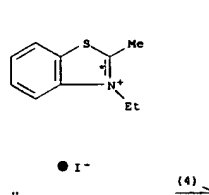
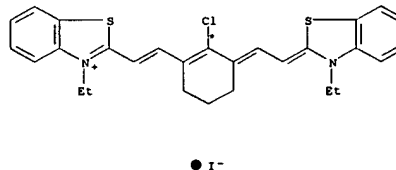
L2 ANSWER 23 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



I  
 YIELD 75%

RX(3) RCT H 3119-93-5, B 61010-04-6  
 PRO I 65303-15-3  
 SOL 71-36-3 BuOH, 71-43-2 Benzene

RX(4) OF 10 ...I + H ==&gt; J



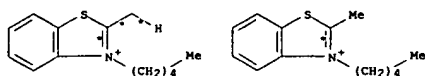
(4) →

L2 ANSWER 23 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

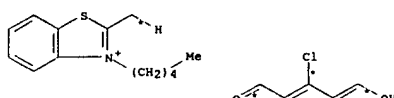
RX(4) RCT I 65303-15-3, H 3119-93-5  
 PRO J 445401-48-9  
 SOL 110-86-1 Pyridine

RX(5) OF 10 3 L + B ==&gt; M

● I<sup>-</sup>● I<sup>-</sup>

L

L

● I<sup>-</sup>

L

B

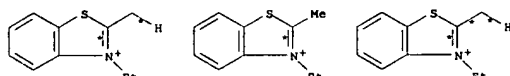
(5)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(5) RCT L 104415-36-3, B 61010-04-6  
 RGT K 110-86-1 Pyridine  
 PRO M 445401-49-0  
 SOL 71-36-3 BuOH, 71-43-2 Benzene

RX(6) OF 10 3 N + B ==&gt; O

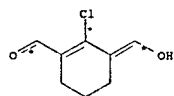
L2 ANSWER 23 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● I<sup>-</sup>● I<sup>-</sup>● I<sup>-</sup>

H

H

H



B

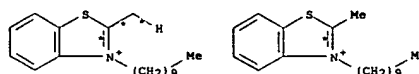
2  
STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(3) RCT H 3119-93-5, B 61010-04-6  
 PRO I 65303-15-3  
 SOL 71-36-3 BuOH, 71-43-2 Benzene

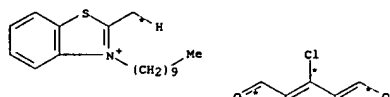
RX(4) RCT I 65303-15-3, H 3119-93-5  
 PRO J 445401-48-9  
 SOL 110-86-1 Pyridine

L2 ANSWER 23 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● I<sup>-</sup>● I<sup>-</sup>

N

N

● I<sup>-</sup>

N

B

(6)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(6) RCT N 445401-54-7, B 61010-04-6  
 RGT K 110-86-1 Pyridine  
 PRO O 445401-50-3  
 SOL 71-36-3 BuOH, 71-43-2 Benzene

RX(10) OF 10 COMPOSED OF RX(3), RX(4)  
 RX(10) 3 M + B ==> J

L2 ANSWER 24 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 137:110523 CASREACT  
 TITLE: Characterization of a novel crown ether-bearing

AUTHOR(S): Tarazi, Leila; Choi, Hoseob; Christian Mason, J.;  
 Sowell, John; Strekowski, Lucjan; Patonay, Gabor

CORPORATE SOURCE: Department of Chemistry, Georgia State University,  
 Atlanta, GA, 30303, USA

SOURCE: Microchemical Journal (2002), 72(1), 55-62  
 CODEN: MICJAN; ISSN: 0026-265X

PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal

LANGUAGE: English

AB The preparation and spectral characteristics of a crown ether-bearing  
 heptamethine cyanine dye (JCM-15C5) and its quenching by lithium ion are  
 reported. The absorbance maximum of the dye is at 776 nm in

acetonitrile. This value matches the output of a com. available laser diode (780 nm),  
 thus making use of such a source practical for excitation. The emission  
 wavelength of the dye in acetonitrile is at 799 nm. It was found that

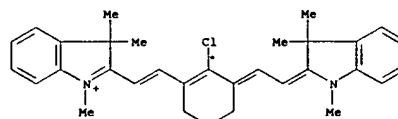
Li<sup>+</sup> ion selectively quenches the fluorescence intensity of JCM-15C5 by the  
 static quenching mechanism. The Stern-Volmer quenching constant (K<sub>sv</sub>)

was 1.17 × 10<sup>7</sup> M<sup>-1</sup> at room temperature. The detection limit for Li<sup>+</sup> ion was  
 7.43 × 10<sup>-2</sup> ppb. The stability constant (K<sub>s</sub>) of the metal-dye complex  
 (determined by fluorometric titration) was 5.40 × 10<sup>7</sup> M<sup>-1</sup>.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR  
 THIS

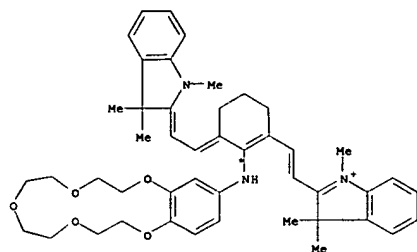
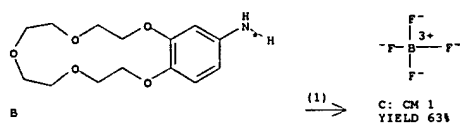
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(1) OF 1 A + B ==&gt; C

● I<sup>-</sup>

A

L2 ANSWER 24 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



C: CM 2  
YIELD 63%

RX(1) RCT A 56289-67-9, B 60835-71-4

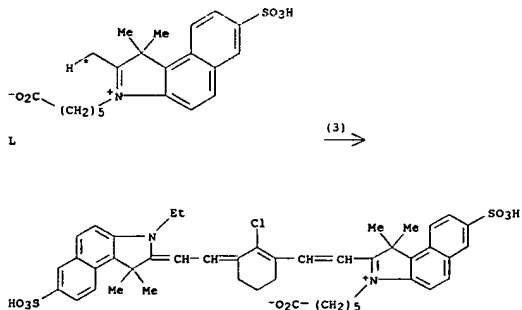
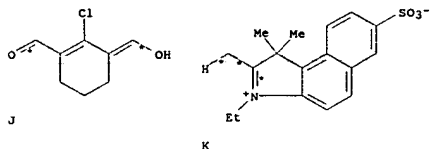
STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
RGT D 16872-11-0 HBF4  
SOL 64-17-5 EtOH, 7732-18-5 Water

PRO C 443661-23-2

L2 ANSWER 25 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS  
FORMAT  
RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(3) OF 6 J + K + L ==> A...

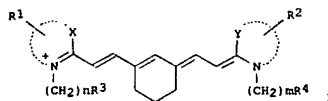


A  
YIELD 24%

RX(3) RCT J 61010-04-6, K 198422-85-4, L 198422-86-5  
RGT M 127-09-3 AcONa  
PRO A 383886-82-6  
SOL 64-19-7 AcOH, 106-24-7 Ac2O

L2 ANSWER 25 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 136:71260 CASREACT  
TITLE: Efficient cyclic-bridged cyanine dyes, their production and their use  
INVENTOR(S): Farooqui, Firdous; Michael, Maged A.; Reddy, M. Parameswara  
PATENT ASSIGNEE(S): Beckman Coulter, Inc., USA  
SOURCE: U.S., 18 pp.  
DOCUMENT TYPE: CODEN: USXXAM  
LANGUAGE: Patent  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6335450	B1	20020101	US 2000-710574	20001109
WO 2002038678	A1	20020516	WO 2001-US45271	20011102
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1337590	A1	20030827	EP 2001-993651	20011102
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
JP 2004523602	T2	20040805	JP 2002-542002	20011102
PRIORITY APPLN. INFO.:			US 2000-710574	20001109
			WO 2001-US45271	20011102
OTHER SOURCE(S):			MARPAT 136:71260	
GI				



AB This invention provides cyclic-bridged dyes (I; each dotted line represents carbon atoms necessary to form a fused substituted or unsubstituted aromatic ring; n = 1-18; m = 1-18; X, Y = S, O, N, CH2 and C(CH3)2; t least one of R1 and R2 comprises a sulfonic acid or sulfonate group attached to the aromatic ring; R3 and R4 are independently selected from the group consisting of carboxyl, activated carboxyl and Me, wherein at least one of R3 and R4 groups is carboxylate or activated carboxylate).

I are useful as fluorescent labels for oligonucleotides. In an example, 2-chloro-1-formyl-3-(hydroxymethyl)cyclohexene was condensed with 3-ethyl-1,2,2-trimethylbenz[e]indolenium-7-sulfonate and 3-(5-carboxypentyl)-1,2,2-trimethylbenz[e]indolenium-7-sulfonate to give

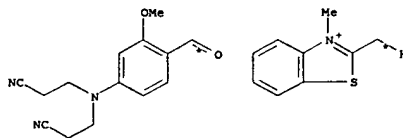
a chlorocyclic monoacid which was then dechlorinated to provide a cyclic bridged cyanine dye which could then be activated for labeling.

L2 ANSWER 26 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 136:71246 CASREACT  
TITLE: Cyanine dyes Part 2  
AUTHOR(S): Jolly, V. S.; Ittyerah, P. I.; Sharma, K. P.  
CORPORATE SOURCE: Chemical Laboratories, St. John's College, Agra, India  
SOURCE: Oriental Journal of Chemistry (2001), 17(2), 275-278  
CODEN: OJCHEG; ISSN: 0970-020X  
PUBLISHER: Oriental Scientific Publishing Co.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB 4-[Bis(2-cyanoethyl)amino]-2-methoxybenzaldehyde and 4-[bis(2-cyanoethyl)amino]-2-ethoxybenzaldehyde (I) on reaction with a number of quaternized heterocyclic amines gave a series of highly colored and lustrous cyanine dyes. Potentialities of the dyes for dyeing cotton, wool, and silk were investigated. The dye obtained by condensation of Fischer's base hydriodide with I dyed cotton, wool, and silk in a bright red shade resistant to washing. One of the dyes showed some photosensitive activity.

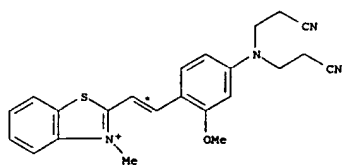
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS  
FORMAT  
RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(6) OF 32 A + M ==> N



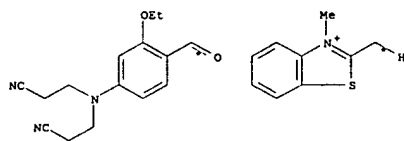
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L2 ANSWER 26 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● I<sup>-</sup>N  
YIELD 47%

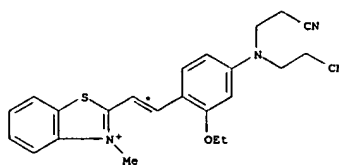
RX(6) RCT A 15310-61-9, M 2785-06-0  
 PRO N 383906-31-8  
 CAT 110-89-4 Piperidine  
 SOL 64-17-5 EtOH

RX(7) OF 32 F + M ==&gt; O

● I<sup>-</sup>

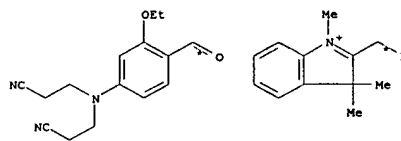
(7) →

L2 ANSWER 26 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● I<sup>-</sup>O  
YIELD 52%

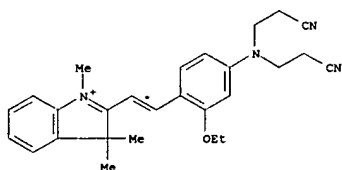
RX(7) RCT F 28006-64-6, M 2785-06-0  
 PRO O 383906-32-9  
 CAT 110-89-4 Piperidine  
 SOL 64-17-5 EtOH

RX(8) OF 32 F + P ==&gt; Q

● I<sup>-</sup>

(8) →

L2 ANSWER 26 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

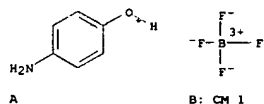
● I<sup>-</sup>Q  
YIELD 84%

RX(8) RCT F 28006-64-6, P 5418-63-3  
 PRO Q 383906-33-0  
 CAT 110-89-4 Piperidine  
 SOL 64-17-5 EtOH

L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

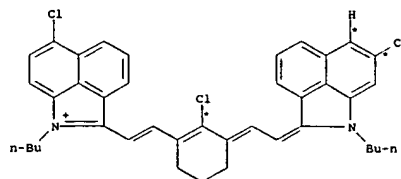
ACCESSION NUMBER: 135:305176 CASREACT  
 TITLE: New heptamethine cyanine reagents for labeling of biomolecules with a near-infrared chromophore  
 AUTHOR(S): Strekowski, Lucjan; Gorecki, Tadeusz; Mason, J. Christian; Lee, Hyeran; Patonay, Gabor  
 CORPORATE SOURCE: Department of Chemistry, Georgia State University, Atlanta, GA, 30303, USA  
 SOURCE: Heterocyclic Communications (2001), 7(2), 117-122  
 CODEN: HCOMEX; ISSN: 0793-0283  
 PUBLISHER: Freund Publishing House Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The syntheses of two fluorescent cyanine dyes (λ<sub>max</sub> = 1033 and 1060 nm in MeOH) with an isothiocyanato function and a succinimidoxycarbonyl-functionalized cyanine dye (λ<sub>max</sub> = 837 nm in MeOH) for labeling of biomols. at amino groups are described.  
 REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(1) OF 14 A + B ==&gt; C...



A

B: CN 1



B: CN 2

(1) →



L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

C: CM 1  
YIELD 30%

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 123-30-8

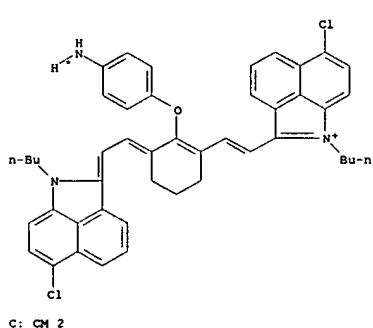
STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 67-66-3 CHCl3STAGE(2)  
RCT B 286472-22-8STAGE(3)  
RGT E 124-38-9 CO2

PRO C 367251-74-9

RX(2) OF 14 ...C + G ==&gt; H

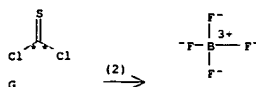


C: CM 1



C: CM 2

L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

H: CM 1  
YIELD 40%

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(2) RCT C 367251-74-9

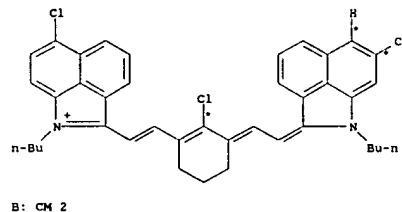
STAGE(1)  
RGT I 497-19-8 Na2CO3  
SOL 68-12-2 DMFSTAGE(2)  
RCT G 463-71-8

PRO H 367251-76-1

RX(3) OF 14 B + K ==&gt; L

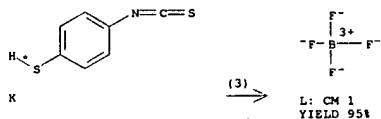


B: CM 1



B: CM 2

L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

L: CM 1  
YIELD 95%

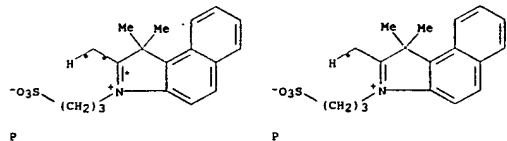
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(3) RCT B 286472-22-8, K 42901-86-0

STAGE(1)  
SOL 68-12-2 DMFSTAGE(2)  
SOL 60-29-7 Et2O

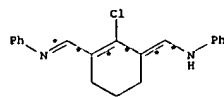
PRO L 367251-78-3

RX(5) OF 14 ...2 P + Q ==&gt; R...



P

P

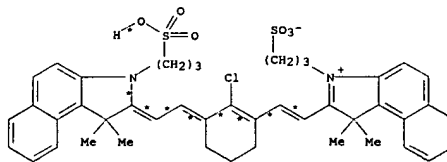


● HCl

(5) →

Q

L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

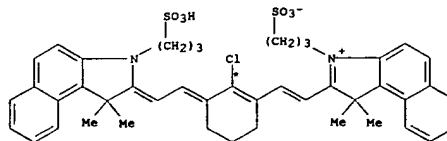
R  
YIELD 85%

RX(5) RCT P 63666-10-4, Q 63857-00-1

STAGE(1)  
RGT S 127-09-3 AcONa  
SOL 64-17-5 EtOHSTAGE(2)  
SOL 60-29-7 Et2O

PRO R 259261-66-0

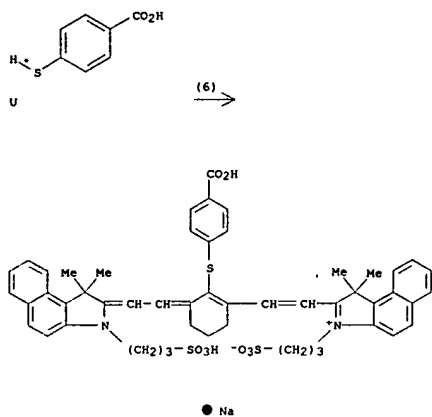
RX(6) OF 14 ...R + U ==&gt; V...



● Na

R

L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

V  
YIELD 90%

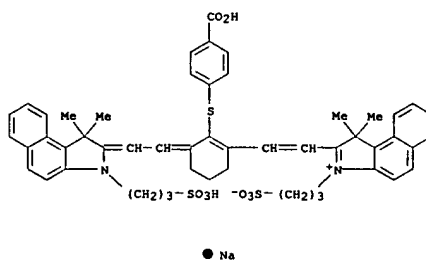
RX(6) RCT R 259261-66-0, U 1074-36-8

STAGE(1)  
SOL 68-12-2 DMFSTAGE(2)  
SOL 60-29-7 Et2O

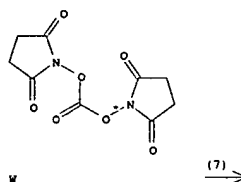
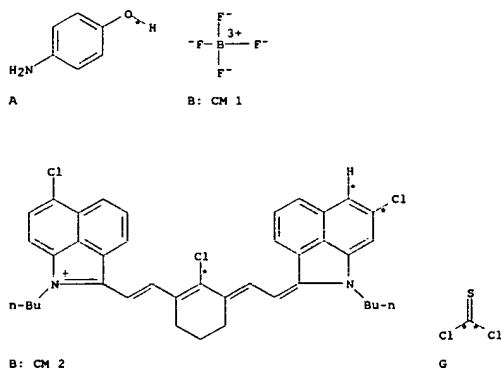
PRO V 367251-79-4

RX(7) OF 14 ...V + W ==&gt; X

L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



V

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*  
PAGE 2-AX  
YIELD 91%RX(7) RCT V 367251-79-4, W 74124-79-1  
PRO X 367251-80-7  
SOL 68-12-2 DMFL2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
NTE literature prepn.RX(8) OF 14 COMPOSED OF RX(1), RX(2)  
RX(8) A + B + G ==> H2  
STEPS  
=>

YIELD 40%

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RX(1) RCT A 123-30-8

STAGE(1)  
RGT D 7646-69-7 NaH  
SOL 67-66-3 CHCl3

L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

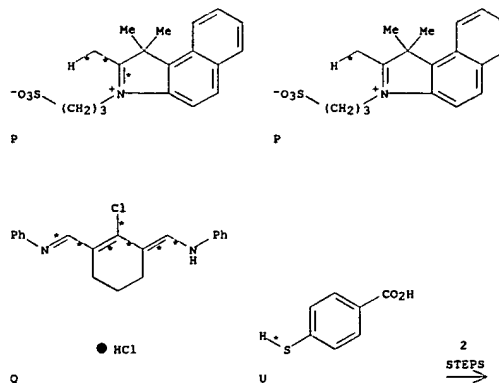
STAGE(2)  
RCT B 286472-22-8STAGE(3)  
RGT E 124-38-9 CO2

PRO C 367251-74-9

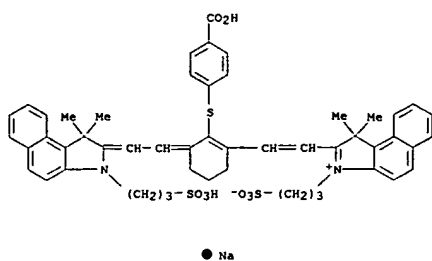
RX(2) RCT C 367251-74-9

STAGE(1)  
RGT I 497-19-8 Na2CO3  
SOL 68-12-2 DMFSTAGE(2)  
RCT G 463-71-8

PRO H 367251-76-1

RX(10) OF 14 COMPOSED OF RX(5), RX(6)  
RX(10) 2 P + Q + U ==> V

L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

V  
YIELD 90%

RX(5) RCT P 63666-10-4, Q 63857-00-1

STAGE(1)  
RGT S 127-09-3 AcONa  
SOL 64-17-5 EtOHSTAGE(2)  
SOL 60-29-7 Et2O

PRO R 259261-66-0

RX(6) RCT R 259261-66-0, U 1074-36-8

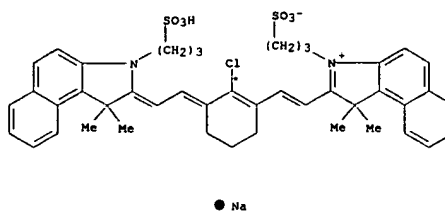
STAGE(1)  
SOL 68-12-2 DMFSTAGE(2)  
SOL 60-29-7 Et2O

PRO V 367251-79-4

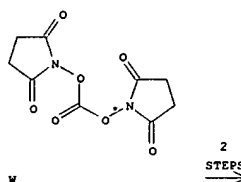
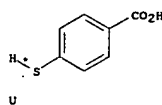
RX(11) OF 14 COMPOSED OF RX(6), RX(7)

RX(11) R + U + W ==&gt; X

L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



R

2  
STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PAGE 2-A

● Na

X  
YIELD 91%

RX(6) RCT R 259261-66-0, U 1074-36-8

STAGE(1)  
SOL 68-12-2 DMFSTAGE(2)  
SOL 60-29-7 Et2O

PRO V 367251-79-4

RX(7) RCT V 367251-79-4, W 74124-79-1

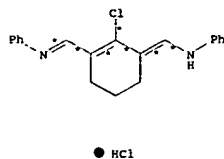
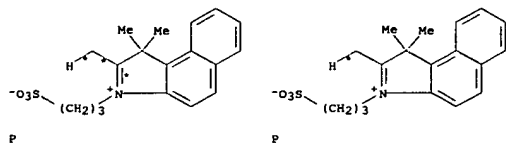
PRO X 367251-80-7

SOL 68-12-2 DMF

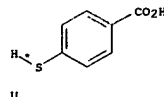
NTE literature prepn.

RX(13) OF 14 COMPOSED OF RX(5), RX(6), RX(7)

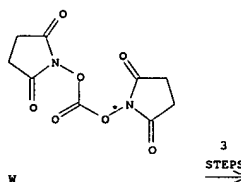
RX(13) 2 P + Q + U + W ==&gt; X



● HCl



L2 ANSWER 27 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

3  
STEPS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-A

● Na

X  
YIELD 91%

RX(5) RCT P 63666-10-4, Q 63857-00-1

STAGE(1)  
RGT S 127-09-3 AcONa  
SOL 64-17-5 EtOHSTAGE(2)  
SOL 60-29-7 Et2O

PRO R 259261-66-0

RX(6) RCT R 259261-66-0, U 1074-36-8

STAGE(1)  
SOL 68-12-2 DMFSTAGE(2)  
SOL 60-29-7 Et2O

PRO V 367251-79-4

RX(7) RCT V 367251-79-4, W 74124-79-1

PRO X 367251-80-7

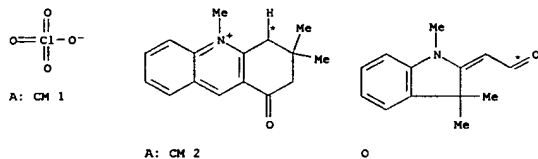
SOL 68-12-2 DMF

NTE literature prepn.

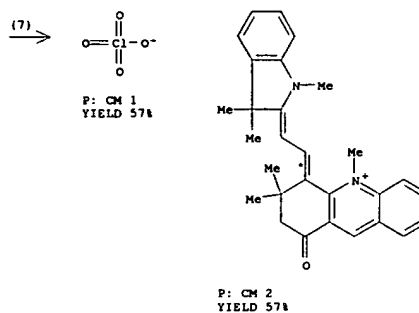
L2 ANSWER 28 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 135:258540 CASREACT  
 TITLE: Reactions of oxotetrahydroacridinium salts via an  
 active  $\alpha$ -methylene group  
 AUTHOR(S): Mel'nik, M. V.  
 CORPORATE SOURCE: Ivano-Frankiv. Derzh. Tekh. Univ. Nafi i Gazu,  
 Ivano-Frankovsk, Ukraine  
 SOURCE: Ukrainskii Khimicheskii Zhurnal (Russian Edition)  
 (2001), 67(3-4), 119-123  
 CODEN: UKZNAU; ISSN: 0041-6045  
 PUBLISHER: Institut Obshchei i Neorganicheskoi Khimii im. V. I.  
 Vernadskogo NAN Ukrainy  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Ukrainian

AB A reaction was carried out between the  $\alpha$ -methylene group of  
 oxotetrahydroacridinium salts and p-dimethylaminobenzaldehyde or  
 1,3,3-trimethyleneformylindoline. Kinetic parameters of styryl dye  
 formation were calculated along with thermodyn. parameters of the dyes.  
 Effect of substituent on the absorption spectra of the dyes was analyzed.

RX(7) OF 11 A + O ==> P

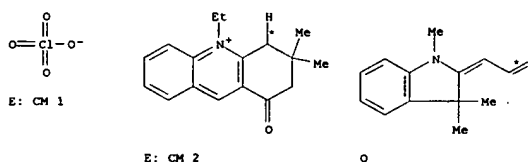


L2 ANSWER 28 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(7) RCT A 361456-87-3, O 84-83-3  
 PRO P 361457-09-2  
 SOL 108-24-7 Ac2O  
 CON 15 minutes, reflux

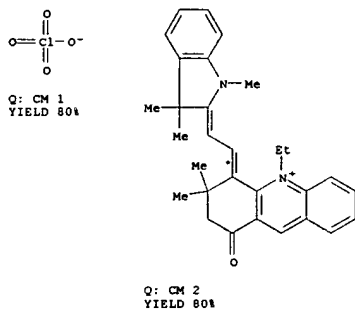
RX(8) OF 11 E + O ==> Q



(8)

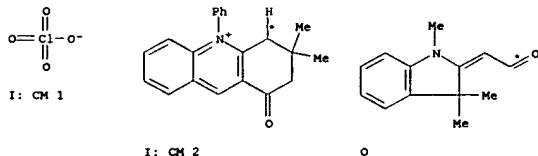
Q: CH 2  
YIELD 80%

L2 ANSWER 28 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

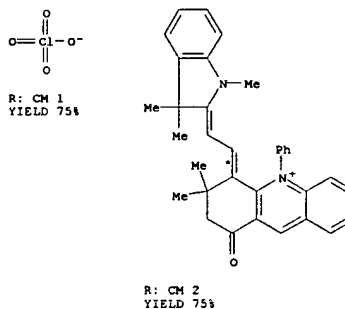


RX(8) RCT E 73143-23-4, O 84-83-3  
 PRO Q 361457-12-7  
 SOL 108-24-7 Ac2O  
 CON 15 minutes, reflux

RX(9) OF 11 I + O ==> R

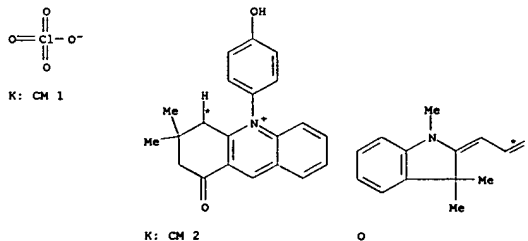


L2 ANSWER 28 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(9) RCT I 73143-25-6, O 84-83-3  
 PRO R 361457-15-0  
 SOL 108-24-7 Ac2O  
 CON 15 minutes, reflux

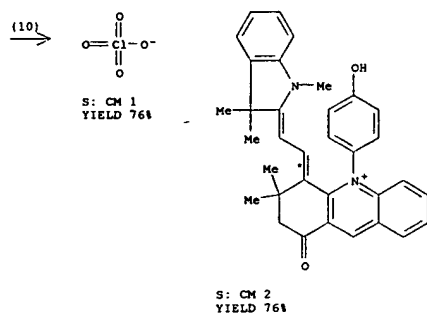
RX(10) OF 11 K + O ==> S



(9)

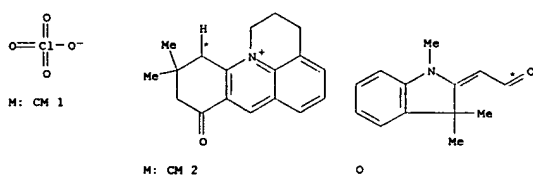
R: CH 2  
YIELD 75%

L2 ANSWER 28 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



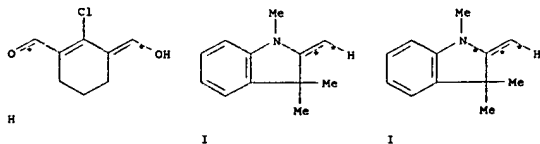
RX(10) RCT K 73143-27-8, O 84-83-3  
PRO S 361457-18-3  
SOL 108-24-7 Ac2O  
CON 15 minutes, reflux

RX(11) OF 11 M + O ==&gt; T

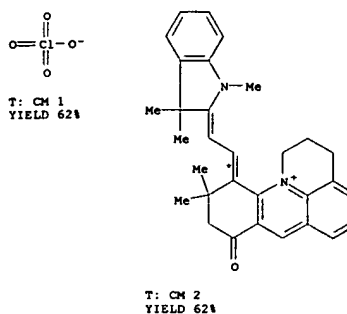
(11)  $\rightarrow$ 

L2 ANSWER 29 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 134:253718 CASREACT  
TITLE: Synthesis and absorption characteristics of two infrared cyanine dyes  
AUTHOR(S): Li, Bin; Tang, Liming; Dong, Hanpeng; Liu, Deshan; Zhou, Qixiang  
CORPORATE SOURCE: Department of Chemical Engineering, Tsinghua University, Beijing, 100084, Peop. Rep. China  
SOURCE: Tsinghua Science and Technology (2000), 5(2), 176-179  
CODEN: TSTEF7; ISSN: 1007-0214  
PUBLISHER: Editorial Board of Journal of Tsinghua University  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Two IR dyes, 1,3,3,1',3',3'-hexamethylindotricarbocyanine iodide (A) and 1,3,3,1',3',3'-hexamethyl-11-chloro-10,12-propylenetricarbocyanine iodide (B), were synthesized and characterized by m.p., elemental anal., and IR and <sup>1</sup>H-NMR spectra. Their electron absorption spectra, laser absorption characteristics, and solubility were investigated. The results showed that A and B have maximum absorption peaks at around 748 and 774 nm, resp., which match well with the wavelength output of a near IR laser diode. The dyes were found to have photoinduced fading during irradiation with the IR laser, especially in the presence of oxygen. However, this procession can be greatly slowed by using a layer of poly(vinyl alc.) to protect the dyes from oxygen. The expts. also showed that the dyes were thermally stable but decayed under strong sunlight. Furthermore, they are easily dissolved in some common solvents.  
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

RX(2) OF 2 H + 2 I ==&gt; J

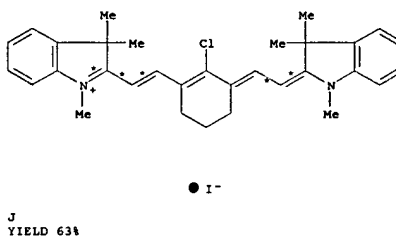
(2)  $\rightarrow$ 

L2 ANSWER 28 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(11) RCT M 361456-94-2, O 84-83-3  
PRO T 361457-21-8  
SOL 108-24-7 Ac2O  
CON 15 minutes, reflux

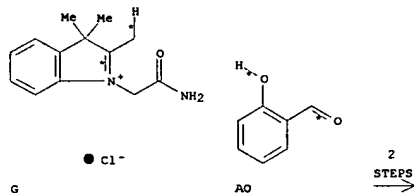
L2 ANSWER 29 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(2) RCT H 61010-04-6, I 118-12-7  
STAGE(1)  
RGT D 127-09-3 AcONa  
STAGE(2)  
RGT E 7681-11-0 KI  
SOL 7732-18-5 Water, 108-24-7 Ac2O  
PRO J 56289-67-9

L2 ANSWER 30 OF 45 CASREACT COPYRIGHT 2006 ACS ON STN  
 ACCESSION NUMBER: 134:147542 CASREACT  
 TITLE: Condensation of 1-carbamoylmethyl-2,3,3-trimethyl-3H-indolium chloride with aromatic aldehydes  
 AUTHOR(S): Sackus, A.; Amankaviciene, V.; Martynaitis, V.  
 CORPORATE SOURCE: Department of Organic Chemistry, Kaunas University of Technology, Kaunas, LT-3028, Lithuania  
 SOURCE: Chemistry of Heterocyclic Compounds (New York) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2000), 36(6), 663-671  
 CODEN: CHCCAL; ISSN: 0009-3122  
 CONSULTANTS BUREAU  
 PUBLISHER: Journal  
 DOCUMENT TYPE: English  
 LANGUAGE: English  
 AB The reaction of 1-carbamoylmethyl-2,3,3-trimethyl-3H-indolium chloride with various aromatic aldehydes in acetic acid and the subsequent workup of the intermediate styrylic derivs. with strong bases yielded 9a-(2-arylethenyl)-1,2,3,9a-tetrahydro-9H-imidazo[1,2-a]indol-2-one derivs. Condensation of the mentioned salt with salicylaldehyde in acidic or basic medium afforded the derivative of 1'-carbamoylmethylspiro[benzopyran-2,2'-indole]. Alkylation of the latter compound with benzyl chloride in the presence of potassium hydroxide gave, 9a-[2-(2-benzyloxyphenyl)ethenyl]-1,2,3,9a-tetrahydro-9H-imidazo[1,2-a]indol-2-one.  
 REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

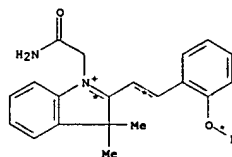
RX(26) OF 28 COMPOSED OF RX(20), RX(22)  
 RX(26) G + AO ==> AT



L2 ANSWER 30 OF 45 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)



AT: CM 1  
 YIELD 54%



AT: CM 2  
 YIELD 54%

RX(20) RCT G 90907-07-6, AO 90-02-8  
 RGT J 64-19-7 AcOH  
 PRO AP 323188-30-3

RX(22) RCT AP 323188-30-3  
 RGT AU 7601-90-3 HClO4  
 PRO AT 323188-33-6  
 SOL 64-17-5 EtOH, 7732-18-5 Water

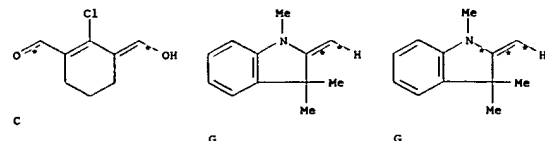
X

L2 ANSWER 31 OF 45 CASREACT COPYRIGHT 2006 ACS ON STN  
 ACCESSION NUMBER: 134:132926 CASREACT  
 TITLE: Cyanine infrared-absorbing compositions and their production  
 INVENTOR(S): Campbell, James Stanley  
 PATENT ASSIGNEE(S): Avecia Limited, UK  
 SOURCE: PCT Int. Appl., 19 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007524	A1	20010201	WO 2000-GB2778	20000719

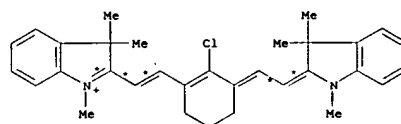
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 PRIORITY APPLN. INFO.: GB 1999-17593 19990728  
 OTHER SOURCE(S): MARPAT 134:132926  
 AB Compsn. comprising cyanine IR-absorbing dyes are provided. The compsn. are substantially free from certain impurities, particularly dimethylcarbamoyl chloride (I). The dyes are prepared by using N-methylformanilide (II) instead of DMF. Thus, I was condensed with cyclohexanone to give 2-chloro-1-formyl-3-(hydroxymethylene)cyclohexene containing no I. The product was then condensed (1:2) with Fischer's base to give a cyanine dye. The production of II using DMF resulted in a product containing 4000 ppb I.  
 REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

RX(2) OF 3 ...C + 2 G ==> H



(2) →

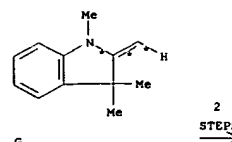
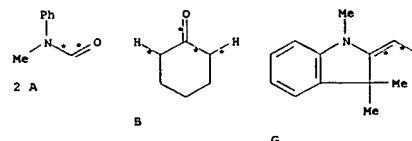
L2 ANSWER 31 OF 45 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)



H Br<sup>-</sup>

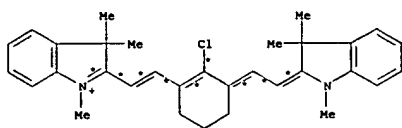
RX(2) RCT C 61010-04-6, G 118-12-7  
 STAGE(1)  
 RGT I 10035-10-6 HBr  
 SOL 108-24-7 Ac2O, 7732-18-5 Water  
 STAGE(2)  
 SOL 7732-18-5 Water  
 PRO H 212964-63-1

RX(3) OF 3 COMPOSED OF RX(1), RX(2)  
 RX(3) 2 A + B + 2 G ==> H



2  
 STEPS →

L2 ANSWER 31 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● Br<sup>-</sup>

H

RX(1) RCT A 93-61-8

STAGE(1)  
RGT D 10025-87-3 POCl<sub>3</sub>  
SOL 141-78-6 AcOEt

STAGE(2)  
RCT B 108-94-1

STAGE(3)  
SOL 7732-18-5 Water

PRO C 61010-04-6

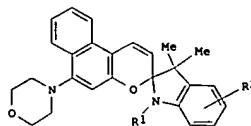
RX(2) RCT C 61010-04-6, G 118-12-7

STAGE(1)  
RGT I 10035-10-6 HBr  
SOL 108-24-7 Ac<sub>2</sub>O, 7732-18-5 Water

STAGE(2)  
SOL 7732-18-5 Water

PRO H 212964-63-1

L2 ANSWER 32 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 134:71510 CASREACT  
TITLE: Photolysis of spiroindolinonaphthopyrans  
AUTHOR(S): Gabbutt, Christopher D.; Hepworth, John D.; Heron, B. Mark; Partington, Steven. M.  
CORPORATE SOURCE: Department of Chemistry, The University of Hull, Hull,  
SOURCE: HU6 7RX, UK  
Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (2000), 345, 323-328  
CODEN: MCLCE9; ISSN: 1058-725X  
PUBLISHER: Gordon & Breach Science Publishers  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

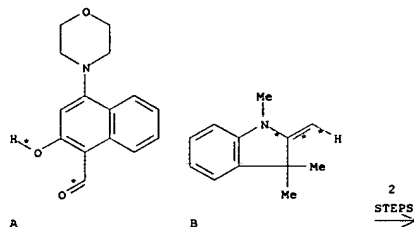


I

AB Some novel amino-substituted spiroindolinonaphthopyrans I (R<sub>1</sub> = Me, CH<sub>2</sub>CHMe<sub>2</sub>, CH<sub>2</sub>CHMe<sub>3</sub>, R<sub>2</sub> = H; R<sub>1</sub> = CH<sub>2</sub>CHMe<sub>2</sub>, R<sub>2</sub> = 5-NHAc; R<sub>1</sub> = Bu, R<sub>2</sub> = 4,5-benzo) have been synthesized. While these compds. exhibit no observable photochromic properties at ambient temperature, protonation in ring opening to give stable, intensely colored dyes. Recyclization and decoloration result on basification.  
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

RX(13) OF 18 COMPOSED OF RX(1), RX(7)  
RX(13) A + B ==> P

L2 ANSWER 32 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



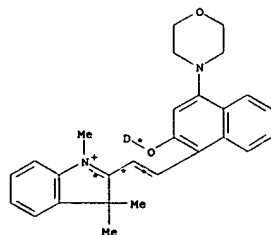
A

B

2 STEPS

-O<sub>3</sub>S-O-D

P: CH 1



P: CH 2

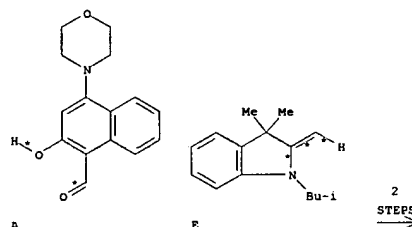
RX(1) RCT A 227295-55-8, B 118-12-7  
PRO C 159595-91-2  
SOL 64-17-5 EtOH

RX(7) RCT C 159595-91-2  
PRO P 315192-60-0  
CAT 7647-01-0 HCl  
SOL 108-88-3 PhMe

RX(14) OF 18 COMPOSED OF RX(2), RX(8)

L2 ANSWER 32 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(14) A + E ==&gt; S



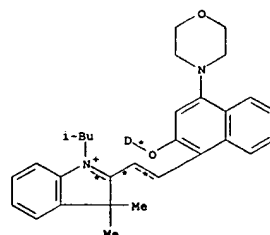
A

E

2 STEPS

-O<sub>3</sub>S-O-D

S: CH 1



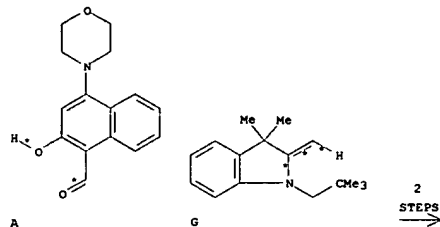
S: CH 2

RX(2) RCT A 227295-55-8, E 159256-80-1  
PRO F 315192-60-0  
SOL 64-17-5 EtOH

RX(8) RCT F 315192-60-0  
PRO S 315192-67-7  
CAT 7647-01-0 HCl  
SOL 108-88-3 PhMe

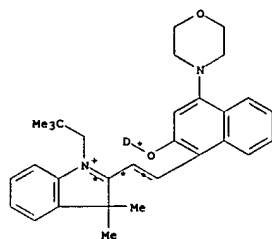
L2 ANSWER 32 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
RX(15) OF 18 COMPOSED OF RX(3), RX(9)  
RX(15) A + G ==> T

(Continued)



-O<sub>3</sub>S-O-D

T: CH 1



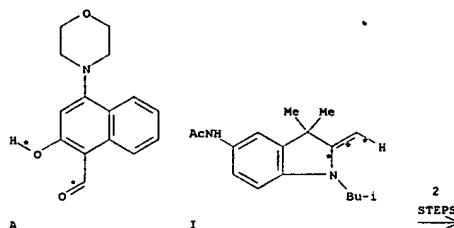
T: CH 2

RX(3) RCT A 227295-55-8, G 159256-81-2  
PRO H 315192-61-1  
SOL 64-17-5 EtOH

RX(9) RCT H 315192-61-1

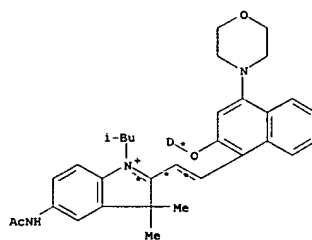
L2 ANSWER 32 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
PRO T 315192-69-9  
CAT 7647-01-0 HCl  
SOL 108-88-3 PhMe

RX(16) OF 18 COMPOSED OF RX(4), RX(10)  
RX(16) A + I ==> U



-O<sub>3</sub>S-O-D

U: CH 1



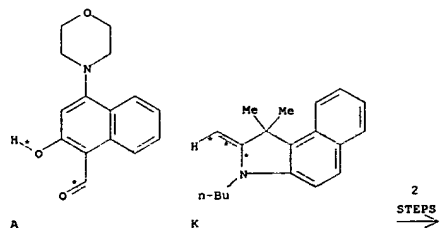
U: CH 2

L2 ANSWER 32 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
RX(4) RCT A 227295-55-8, I 315192-58-6  
PRO J 315192-62-2  
SOL 64-17-5 EtOH

(Continued)

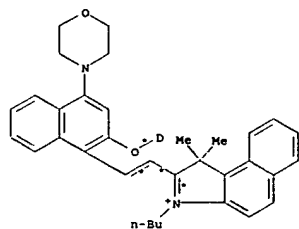
RX(10) RCT J 315192-62-2  
PRO U 315192-71-3  
CAT 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
SOL 67-64-1 Me<sub>2</sub>CO

RX(17) OF 18 COMPOSED OF RX(5), RX(11)  
RX(17) A + K ==> X



-O<sub>3</sub>S-O-D

X: CH 1



X: CH 2

L2 ANSWER 32 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
RX(5) RCT A 227295-55-8, K 315192-59-7  
PRO L 315192-63-3  
SOL 64-17-5 EtOH

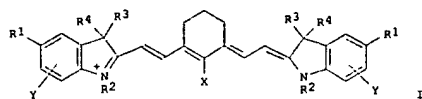
RX(11) RCT L 315192-63-3  
PRO X 315192-73-8  
CAT 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
SOL 67-64-1 Me<sub>2</sub>CO



L2 ANSWER 33 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 134:57944 CASREACT  
 TITLE: Near-IR-absorbing polymethine dyes, their production and their use  
 INVENTOR(S): Fujita, Shigeo; Sasaki, Nobuaki; Iwasaki, Yasuhisa; Chichishi, Keiki  
 PATENT ASSIGNEE(S): Yamamoto Chemicals, Inc., Japan  
 SOURCE: Eur. Pat. Appl., 53 pp.  
 CODEN: EPXKDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1063231	A1	20001227	EP 2000-305192	20000620
EP 1063231	B1	20050511		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2001064255	A2	20010313	JP 2000-184294	20000620
JP 3606165	B2	20050105		
US 6342335	B1	20020129	US 2000-598044	20000620
US 39105	E	20060523	US 2004-763075	20040123
			JP 1999-174235	19990621

PRIORITY APPL. INFO.:  
 OTHER SOURCE(S): MARPAT 134:57944  
 GI



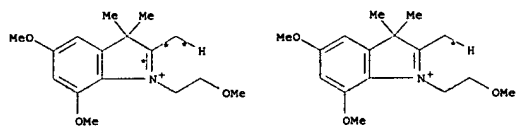
AB The invention provides near-IR-absorbing dyes (I: R1 = optionally substituted alkoxy; R2 = optionally substituted alkyl; R3, R4 = lower alkyl; R3R4 together may form a ring; X = H, halogen, substituted amino; Y = optionally substituted alkoxy or alkyl; Z = charge-neutralizing ion) with high light-to-heat conversion efficiency and high sensitivity to lasers whose emission bands are within the range of 750 nm to 900 nm. I are produced using the appropriate X-substituted cyclohexene and indolium compds. and may be used in original plates for direct printing plate making.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

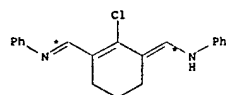
FORMAT

L2 ANSWER 33 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 PRO C 313904-13-3

RX(2) OF 8 2 H + I ==> J

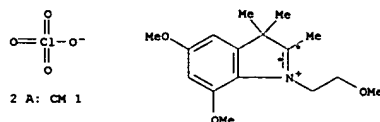


H I

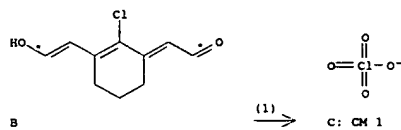


I (2) →

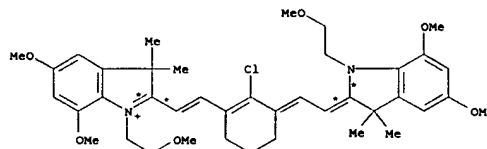
L2 ANSWER 33 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 RX(1) OF 8 2 A + B ==> C



2 A: CM 1 2 A: CM 2



B (1) → C: CM 1



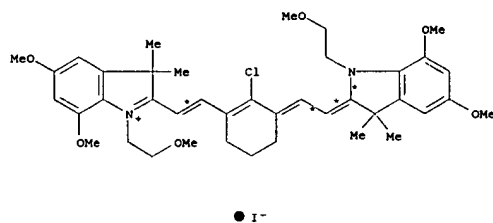
C: CM 2

RX(1) RCT A 313904-22-4, B 273198-39-3

STAGE(1)  
 RGT D 127-08-2 AcOK  
 SOL 108-24-7 Ac2O

STAGE(2)  
 RGT E 7778-74-7 KClO4  
 SOL 7732-18-5 Water

L2 ANSWER 33 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



J

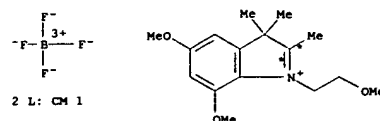
RX(2) RCT H 313904-23-5, I 63857-00-1

STAGE(1)  
 RGT D 127-08-2 AcOK  
 SOL 108-24-7 Ac2O

STAGE(2)  
 RGT K 7681-11-0 KI  
 SOL 7732-18-5 Water

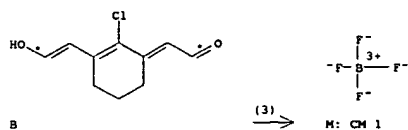
PRO J 313904-14-4

RX(3) OF 8 2 L + B ==> M



2 L: CM 1 2 L: CM 2

L2 ANSWER 33 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



M: CM 2

RX (3) RCT L 313984-24-6, B 273198-39-3

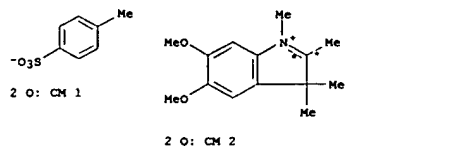
STAGE (1)  
RGT D 127-08-2 AcOK  
SOL 108-24-7 Ac2O

STAGE (2)  
RGT N 14075-53-7 KBF4  
SOL 7732-18-5 Water

PRO M 313984-15-5

RX (4) OF 8 2 O + B ==&gt; P

L2 ANSWER 33 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



P: CM 2

RX (4) RCT O 313984-26-8, B 273198-39-3

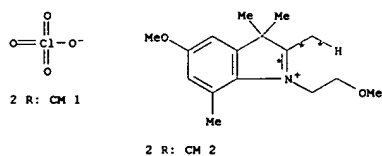
STAGE (1)  
RGT D 127-08-2 AcOK  
SOL 108-24-7 Ac2O

STAGE (2)  
RGT Q 104-15-4 TsOH  
SOL 7732-18-5 Water

PRO P 313984-17-7

RX (5) OF 8 2 R + I ==&gt; S

L2 ANSWER 33 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



S: CM 1

S: CM 2

RX (5) RCT R 313984-28-0, I 63857-00-1

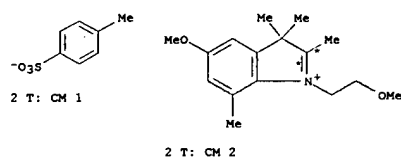
STAGE (1)  
RGT D 127-08-2 AcOK  
SOL 108-24-7 Ac2O

STAGE (2)  
RGT E 7778-74-7 KClO4  
SOL 7732-18-5 Water

L2 ANSWER 33 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO S 313984-18-8

RX (6) OF 8 2 T + B ==&gt; U



U: CM 1

U: CM 2

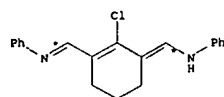
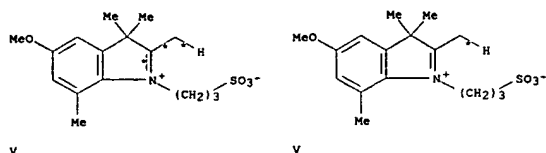
RX (6) RCT T 313984-29-1, B 273198-39-3

STAGE (1)  
RGT D 127-08-2 AcOK  
SOL 108-24-7 Ac2O

STAGE (2)  
RGT Q 104-15-4 TsOH  
SOL 7732-18-5 Water

L2 ANSWER 33 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
PRO U 313984-19-9

RX(7) OF 8 2 V + I ==> W

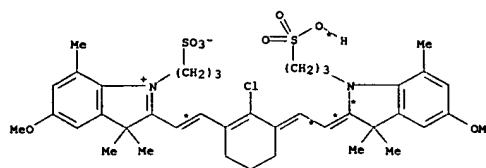


● HCl

(7) →

I

L2 ANSWER 33 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● Na

W

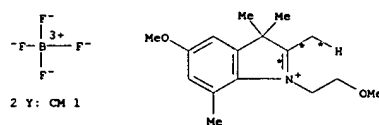
RX(7) RCT V 313984-30-4, I 63857-00-1

STAGE(1)  
RGT D 127-08-2 AcOK  
SOL 108-24-7 Ac2O

STAGE(2)  
SOL 67-63-0 Me2CHOH

PRO W 313984-20-2

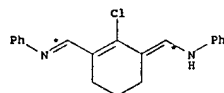
RX(8) OF 8 2 Y + I ==> Z



2 Y: CM 1

2 Y: CM 2

L2 ANSWER 33 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



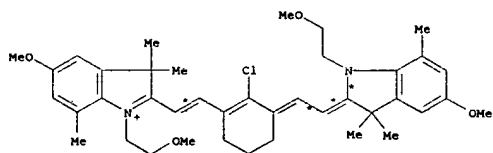
● HCl

(8) →



Z: CM 1

I



Z: CM 2

RX(8) RCT Y 313984-31-5, I 63857-00-1

STAGE(1)  
RGT D 127-08-2 AcOK  
SOL 108-24-7 Ac2O

STAGE(2)  
RGT N 14075-53-7 KBF4  
SOL 7732-18-5 Water

PRO Z 285568-69-6

L2 ANSWER 34 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 134:5904 CASREACT  
TITLE: The addition reaction of hydroxide or ethoxide ion with benzindolium heptamethine cyanine dyes  
AUTHOR(S): Strekowski, Lucjan; Mason, J. Christian; Britton, Jonathan E.; Lee, Hyeran; Van Aken, Koen; Patonay, Gabor  
CORPORATE SOURCE: Department of Chemistry, Georgia State University, Atlanta, GA, 30303, USA  
SOURCE: Dyes and Pigments (2000), 46(3), 163-168  
CODEN: DYPIDX; ISSN: 0143-7208  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB This paper pertains to a nucleophilic addition reaction at the C2 atom of a benz[c]indolium or 3,3-dimethyl-1H-benz[e]indolium subunit of the corresponding near-IR heptamethine cyanine that contains a chlorine atom at the central meso position of the chromophore. An important finding is that the efficient SRN1 replacement of the chloro substituent in such dyes

is completely suppressed in the reactions (i) of hydroxide and ethoxide ions, both of which are poor single electron donors and (ii) conducted in aqueous alc., a medium that does not promote single electron transfer.

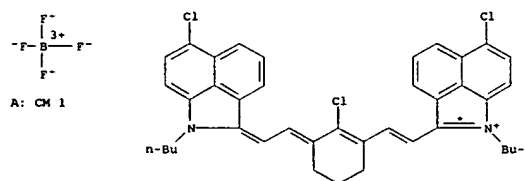
The adducts produced were isolated and characterized by elemental anal., 1H NMR, and 13C NMR. The NIR-absorbing parent dye is regenerated quant.

upon treatment of the corresponding adduct with a weak acid, including silica gel.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS

FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

RX(1) OF 3 A + B ==> C

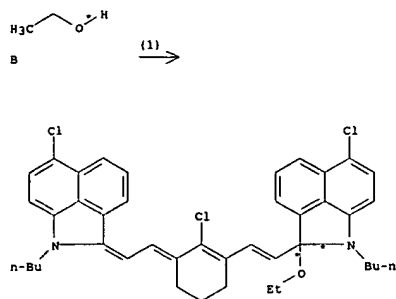


A: CM 1

A: CM 2

L2 ANSWER 34 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

C  
YIELD 79%

RX(1) RCT A 155613-98-2, B 64-17-5

STAGE(1)

RGT D 1310-58-3 KOH

SOL 64-17-5 EtOH, 7732-18-5 Water

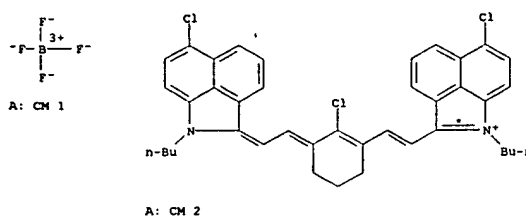
STAGE(2)

SOL 7732-18-5 Water

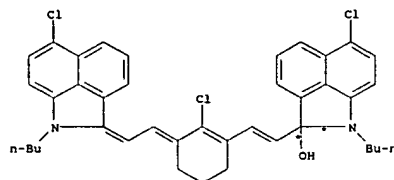
PRO C 308810-27-7

RX(2) OF 3 A ==&gt; F

L2 ANSWER 34 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



(2)

F  
YIELD 90%

RX(2) RCT A 155613-98-2

STAGE(1)

RGT D 1310-58-3 KOH

SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

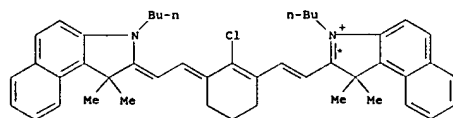
SOL 7732-18-5 Water

PRO F 308810-28-8

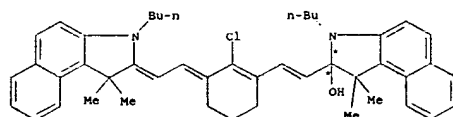
L2 ANSWER 34 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

RX(3) OF 3 H ==&gt; I

H  
● I<sup>-</sup>

(3)

I  
YIELD 93%

RX(3) RCT H 308810-29-9

STAGE(1)

RGT D 1310-58-3 KOH

SOL 67-56-1 MeOH, 7732-18-5 Water

STAGE(2)

SOL 7732-18-5 Water

PRO I 308810-30-2

L2 ANSWER 35 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

132:347777 CASREACT

TITLE:

Studies Directed toward the Synthesis of

CRYPTOHEPTINE

AUTHOR(S):

Zhang, Pingsheng; Blierer, Donald E.

CORPORATE SOURCE:

Shaman Pharmaceuticals, South San Francisco, CA,

94080-4812, USA

SOURCE:

Journal of Natural Products (2000), 63(5), 643-645

CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Synthesis of 5,10-dihydro-10-methylindolo[3,2-b][1]benzazepin-12(11H)-one (I), an isomer of the reported structure for cryptoheptine (II), is presented. Attempts to convert I to II led to 10-methylindolo[3,2-b][1]benzazepin-12-one (III), an oxidation product of I and presumably

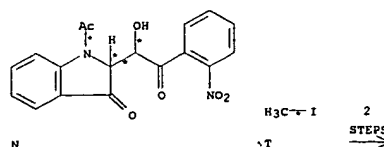
II. These results highlight the potential instability of cryptoheptine (II) and cast doubt on its proposed structure.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

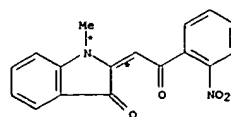
RX(10) OF 21 COMPOSED OF RX(4), RX(5)

RX(10) N + T ==&gt; A



N

$\text{H}_3\text{C}-\text{O}^-\text{H} \xrightarrow{2 \text{ STEPS}}$   
 T

A  
YIELD 83%

L2 ANSWER 35 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(4) RCT N 269077-06-7

STAGE(1)

RGT Q 7647-01-0 HCl

SOL 7732-18-5 Water, 109-99-9 THF

STAGE(2)

RGT R 144-55-8 NaHCO<sub>3</sub>

SOL 7732-18-5 Water

PRO P 25410-92-8

RX(5) RCT P 25410-92-8

STAGE(1)

RGT U 7646-69-7 NaH

SOL 68-12-2 DMF

STAGE(2)

RCT T 74-88-4

PRO A 269077-07-8

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

127:231448

CASREACT

TITLE:

Functionalized Tricarbocyanine Dyes as Near-Infrared

Fluorescent Probes for Biomolecules

Flanagan, James H., Jr.; Khan, Shaheer H.; Menchen,

Steve; Soper, Steven A.; Hammer, Robert P.

Department of Chemistry, Louisiana State University,

Baton Rouge, LA, 70803-1804, USA

SOURCE:

Bioconjugate Chemistry (1997), 8(5), 751-756

CODEN: BOCHE5; ISSN: 1043-1802

American Chemical Society

PUBLISHER:

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB

The syntheses of 3 novel functionalized tricarbocyanine dyes are described. These dyes containing isothiocyanate and succinimidyl ester functional groups are reactive toward primary amines and can be used as fluorescent probes for biol. pertinent compds. such as amino acids and functionalized dideoxynucleotides. The absorption and fluorescence

maxima

occur in the near-IR region of the spectrum (770-820 nm). The

succinimidyl

ester proved to be very sensitive to hydrolysis and was generated in situ to label amino acids and alkyl amines. The isothiocyanates were less susceptible to hydrolysis and were conjugated using organic modified [40% (volume/volume) acetonitrile] buffers to amino acids. A dye with an

alkyl

isothiocyanate moiety showed conjugation to amino-functionalized dideoxynucleotide triphosphates.

REFERENCE COUNT:

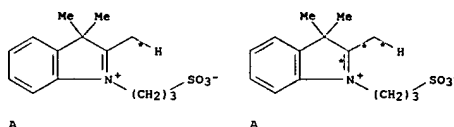
27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR

THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

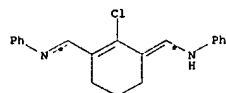
RX(1) OF 44 ...2 A + B ==&gt; C...



A

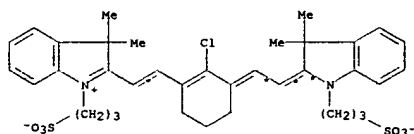
A

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



● HCl

(1) →

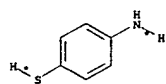


C

YIELD 52%

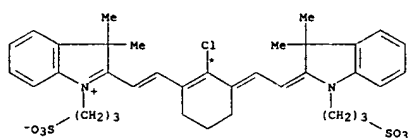
RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(2) OF 44 ...F + C + G ==&gt; H

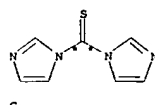


F

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

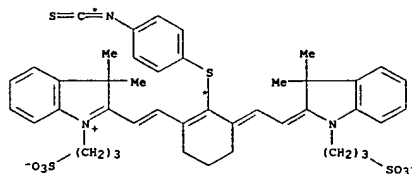


C



G

(2) →



H

YIELD 29%

RX(2) RCT F 1193-02-8, C 160846-41-3

STAGE(1)

SOL 68-12-2 DMF

STAGE(2)

RCT G 6160-65-2

STAGE(3)

SOL 60-29-7 Et2O

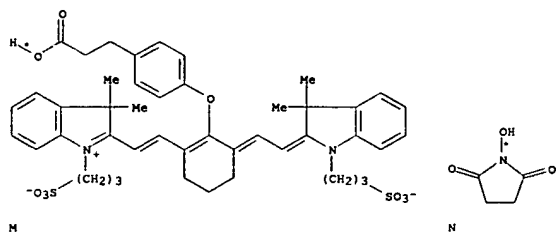
L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(4)

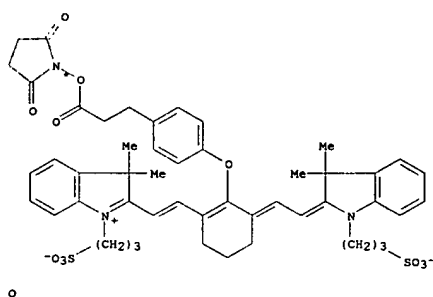
SOL 7732-18-5 Water, 67-56-1 MeOH

PRO H 160846-42-4

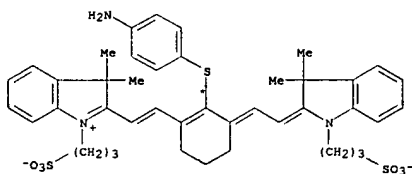
RX(3) OF 44 ...M + N ==&gt; O



(3)



L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



YIELD 50%

RX(6) RCT F 1193-02-8

STAGE(1)

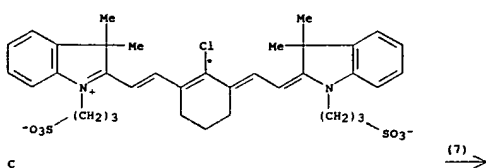
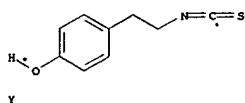
SOL 68-12-2 DMF

STAGE(2)

RCT C 160846-41-3

PRO X 195382-11-7

RX(7) OF 44 ...Y + C ==&gt; Z



(7)

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(3) RCT M 195382-12-8, N 6066-82-6

STAGE(1)

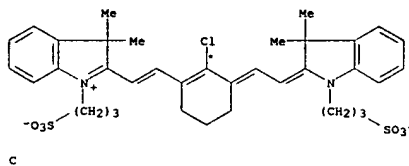
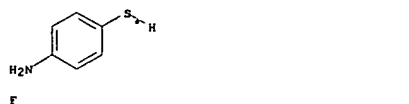
SOL 68-12-2 DMF

STAGE(2)

RGT P 538-75-0 DCC

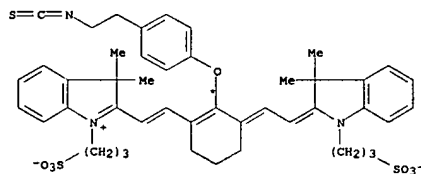
PRO O 195382-09-3

RX(6) OF 44 ...F + C ==&gt; X...



(6)

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



YIELD 32%

RX(7) RCT Y 60114-04-7

STAGE(1)

RGT AA 7646-69-7 NaH

SOL 68-12-2 DMF

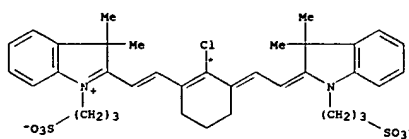
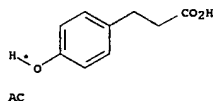
STAGE(2)

RCT C 160846-41-3

SOL 68-12-2 DMF

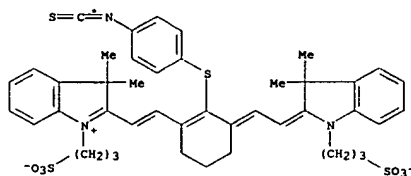
PRO Z 195382-08-2

RX(9) OF 44 ...AC + C ==&gt; M...



(9)

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



H  
YIELD 39%

RX(10) RCT X 195382-11-7

STAGE (1)  
RGT AE 497-19-8 Na2CO3  
SOL 68-12-2 DMF

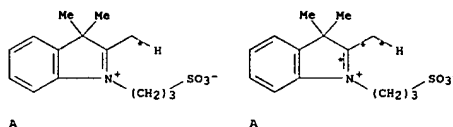
STAGE (2)  
RCT AD 463-71-8

PRO H 160846-42-4

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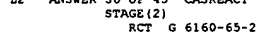
RX(11) OF 44 COMPOSED OF RX(1), RX(2)
RX(11)      2 A  + B  + F  + G  ==>  H

```



(10)

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



STAGE (3)  
SOL 60-29-7 Et2O

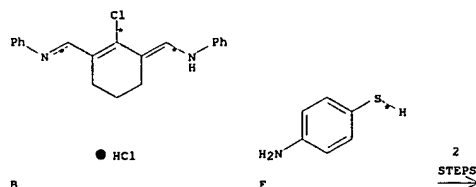
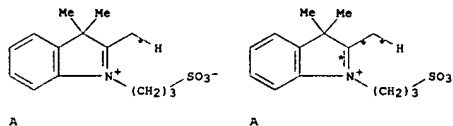
STAGE (4)  
SOL 7732-18-5 Water, 67-56-1 MeOH

PRO H 160846-42-4

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RX(12) OF 44 COMPOSED OF RX(1), RX(6)
RX(12)      2 A + B + F ==> X

```



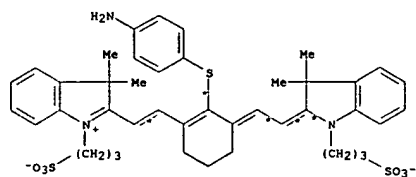
H  
YIELD 294

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(2) RCT F 1193-02-8, C 160846-41-3  
STAGE(1)  
SOL 68-12-2 DMF

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

X  
YIELD 50%

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

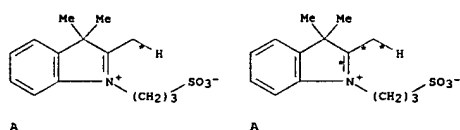
RX(6) RCT F 1193-02-8

STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3

PRO X 195382-11-7

RX(13) OF 44 COMPOSED OF RX(1), RX(7)  
RX(13) 2 A + B + Y ==> X

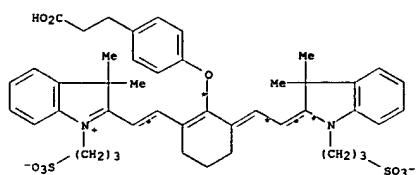
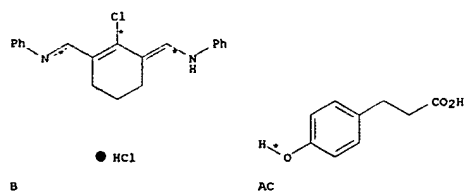
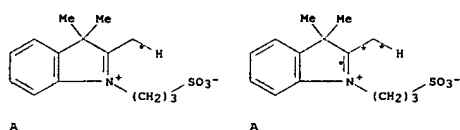


L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

PRO Z 195382-08-2

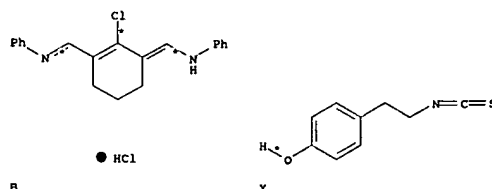
RX(14) OF 44 COMPOSED OF RX(1), RX(9)  
RX(14) 2 A + B + AC ==> M

M  
YIELD 31%

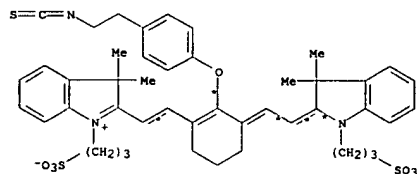
RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



2  
STEPS

Z  
YIELD 32%

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(7) RCT Y 60114-04-7

STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3  
SOL 68-12-2 DMF

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

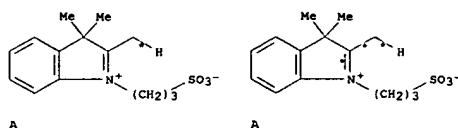
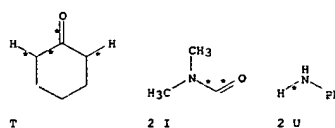
RX(9) RCT AC 501-97-3

STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

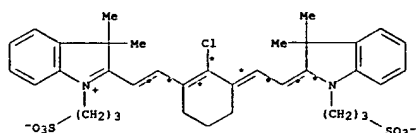
STAGE(2)  
RCT C 160846-41-3

PRO M 195382-12-8

RX(16) OF 44 COMPOSED OF RX(5), RX(1)  
RX(16) T + 2 I + 2 U + 2 A ==> C



2  
STEPS

C  
YIELD 52%

RX(5) RCT T 108-94-1, I 68-12-2



L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(1)  
RGT V 10025-87-3 POC13  
SOL 68-12-2 DMF

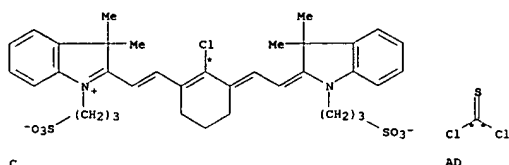
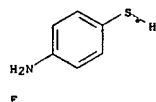
STAGE(2)  
RGT U 62-53-3  
SOL 64-17-5 EtOH

STAGE(3)  
RGT W 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO B 195382-10-6

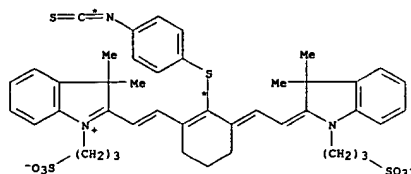
RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(17) OF 44 COMPOSED OF RX(6), RX(10)  
RX(17) F + C + AD ==> H



2  
STEPS  
=>

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



YIELD 39%

RX(6) RCT F 1193-02-8

STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3

PRO X 195382-11-7

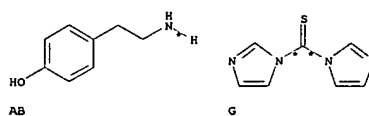
RX(10) RCT X 195382-11-7

STAGE(1)  
RGT AE 497-19-8 Na2CO3  
SOL 68-12-2 DMF

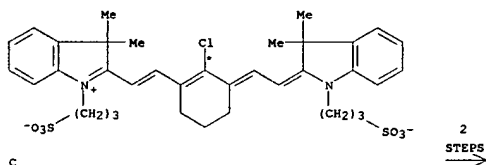
STAGE(2)  
RCT AD 463-71-8

PRO H 160846-42-4

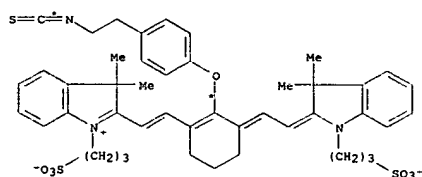
RX(18) OF 44 COMPOSED OF RX(8), RX(7)  
RX(18) AB + G + C ==> Z



L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



2  
STEPS  
=>



YIELD 32%

RX(8) RCT AB 51-67-2

STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
RCT G 6160-65-2

PRO Y 60114-04-7

RX(7) RCT Y 60114-04-7

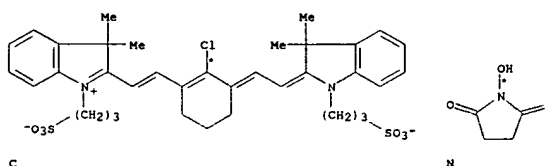
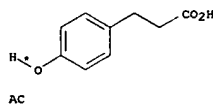
STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3  
SOL 68-12-2 DMF

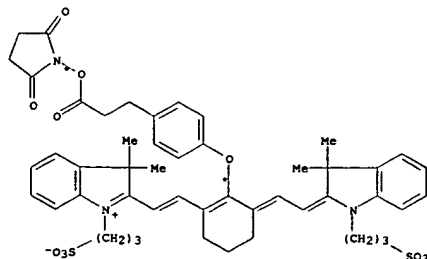
PRO Z 195382-08-2

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(19) OF 44 COMPOSED OF RX(9), RX(3)  
RX(19) AC + C + N ==> O



2  
STEPS  
=>



L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
RX(9) RCT AC 501-97-3

STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3

PRO M 195382-12-8

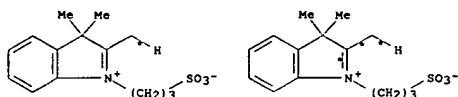
RX(3) RCT M 195382-12-8, N 6066-82-6

STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
RGT P 538-75-0 DCC

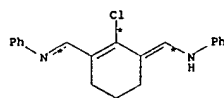
PRO O 195382-09-3

RX(20) OF 44 COMPOSED OF RX(1), RX(6), RX(10)  
RX(20) 2 A + B + F + AD ==> H



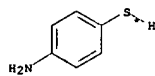
A

A



● HCl

B



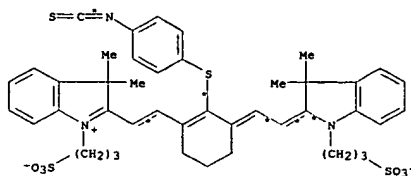
F



AD

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

3  
STEPS  
→



H  
YIELD 39%

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8

STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3

PRO X 195382-11-7

RX(10) RCT X 195382-11-7

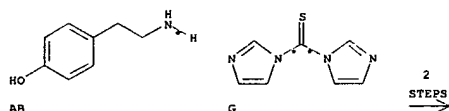
STAGE(1)  
RGT AE 497-19-8 Na2CO3  
SOL 68-12-2 DMF

STAGE(2)  
RCT AD 463-71-8

PRO H 160846-42-4

RX(21) OF 44 COMPOSED OF REACTION SEQUENCE RX(8), RX(7)  
AND REACTION SEQUENCE RX(1), RX(7)

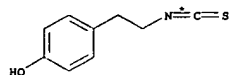
L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
...AB + G ==> Y...  
...2 A + B + Y ==> Z



AB

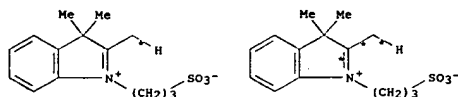
G

2  
STEPS  
→



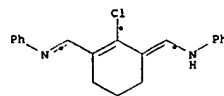
Y

START NEXT REACTION SEQUENCE



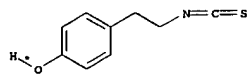
A

A



● HCl

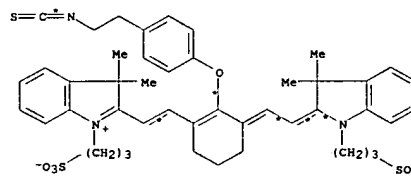
B



Y

2  
STEPS  
→

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



Z  
YIELD 32%

RX(8) RCT AB 51-67-2

STAGE(1)  
SOL 68-12-2 DMF

STAGE(2)  
RCT G 6160-65-2

PRO Y 60114-04-7

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(7) RCT Y 60114-04-7

STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

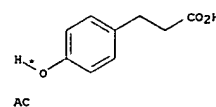
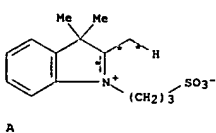
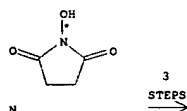
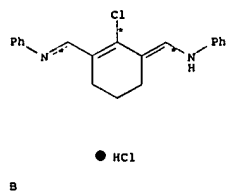
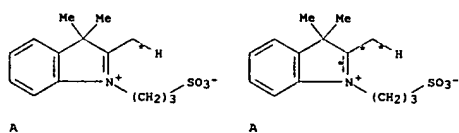
STAGE(2)  
RCT C 160846-41-3  
SOL 68-12-2 DMF

PRO Z 195382-08-2

RX(22) OF 44 COMPOSED OF RX(1), RX(9), RX(3)  
RX(22) 2 A + B + AC + N ==> O

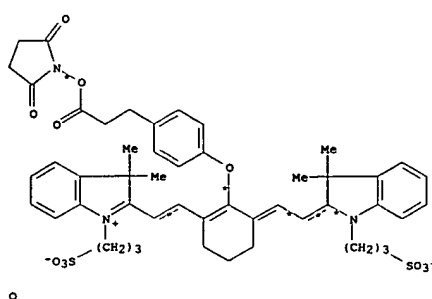
L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

RX(9) RCT AC 501-97-3

STAGE(1)  
 RGT AA 7646-69-7 NaH  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT C 160846-41-3

PRO M 195382-12-8

RX(3) RCT M 195382-12-8, N 6066-82-6

STAGE(1)  
 SOL 68-12-2 DMF

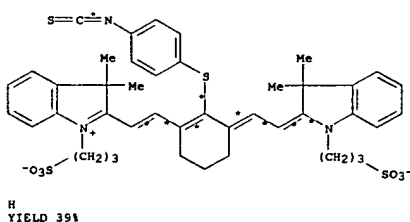
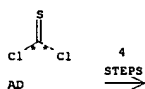
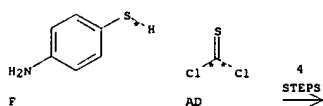
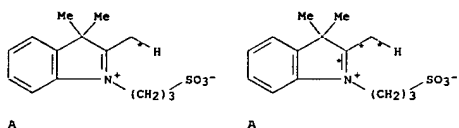
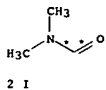
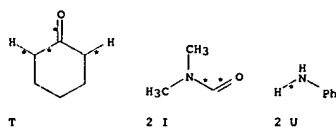
STAGE(2)  
 RGT P 538-75-0 DCC

PRO O 195382-09-3

RX(26) OF 44 COMPOSED OF RX(5), RX(1), RX(6), RX(10)  
 RX(26) T + 2 I + 2 U + 2 A + F + AD ==> H

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

RGT V 10025-87-3 POC13  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT U 62-53-3  
 SOL 64-17-5 EtOH

STAGE(3)  
 RGT W 7647-01-0 HCl  
 SOL 7732-18-5 Water

PRO B 195382-10-6

RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8

STAGE(1)  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT C 160846-41-3

PRO X 195382-11-7

RX(10) RCT X 195382-11-7

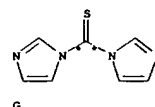
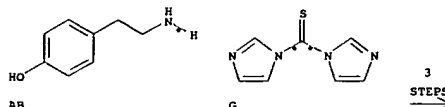
STAGE(1)  
 RGT AE 497-19-8 Na2CO3  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT AD 463-71-8

PRO H 160846-42-4

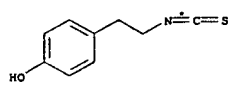
RX(27) OF 44 COMPOSED OF REACTION SEQUENCE RX(8), RX(7)  
 AND REACTION SEQUENCE RX(5), RX(1), RX(7)

...AB + G ==> Y...  
 ...T + 2 I + 2 U + 2 A + Y ==> B

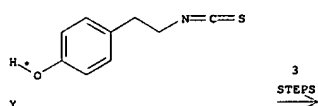
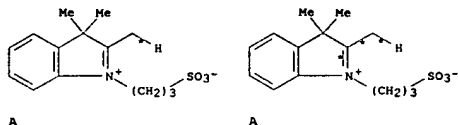
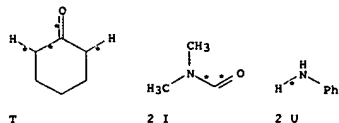


3  
 STEPS

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



START NEXT REACTION SEQUENCE



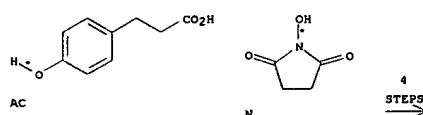
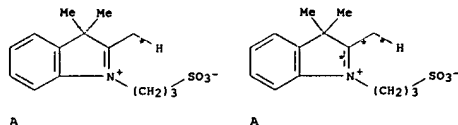
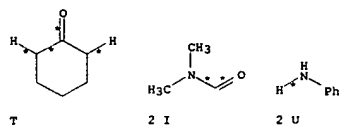
L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE (2)  
RCT C 160846-41-3  
SOL 68-12-2 DMF

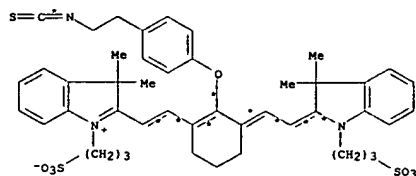
PRO Z 195382-08-2

RX (28) OF 44 COMPOSED OF RX (5), RX (1), RX (9), RX (3)

RX (28) T + 2 I + 2 U + 2 A + AC + N =====&gt; O



L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



YIELD 32%

RX (8) RCT AB 51-67-2

STAGE (1)  
SOL 68-12-2 DMF

STAGE (2)  
RCT G 6160-65-2

PRO Y 60114-04-7

RX (5) RCT T 108-94-1, I 68-12-2

STAGE (1)  
RGT V 10025-87-3 POC13  
SOL 68-12-2 DMF

STAGE (2)  
RCT U 62-53-3  
SOL 64-17-5 EtOH

STAGE (3)  
RGT W 7647-01-0 HCl  
SOL 7732-18-5 Water

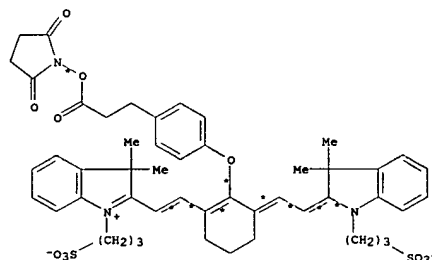
PRO B 195382-10-6

RX (1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX (7) RCT Y 60114-04-7

STAGE (1)  
RGT AA 7646-69-7 NaH

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX (5) RCT T 108-94-1, I 68-12-2

STAGE (1)  
RGT V 10025-87-3 POC13  
SOL 68-12-2 DMF

STAGE (2)  
RCT U 62-53-3  
SOL 64-17-5 EtOH

STAGE (3)  
RGT W 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO B 195382-10-6

RX (1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX (9) RCT AC 501-97-3

STAGE (1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

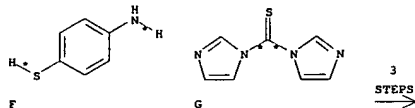
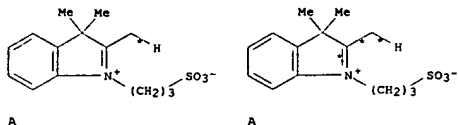
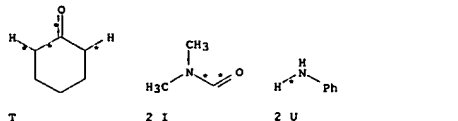
STAGE (2)  
RCT C 160846-41-3

PRO M 195382-12-8

RX (3) RCT M 195382-12-8, N 6066-82-6

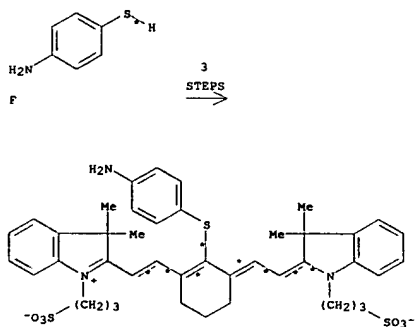
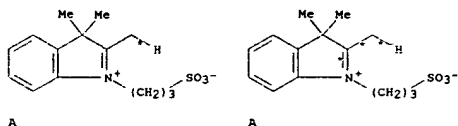
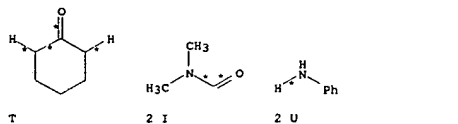
L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 STAGE(1)  
 SOL 68-12-2 DMF  
 STAGE(2)  
 RGT P 538-75-0 DCC  
 PRO O 195382-09-3

RX(34) OF 44 COMPOSED OF RX(5), RX(1), RX(2)  
 RX(34) T + 2 I + 2 U + 2 A + F + G ==> H



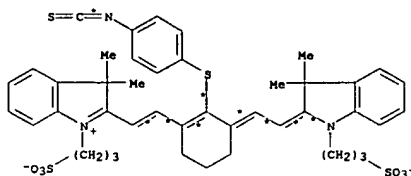
L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 PRO H 160846-42-4

RX(35) OF 44 COMPOSED OF RX(5), RX(1), RX(6)  
 RX(35) T + 2 I + 2 U + 2 A + F ==> X



X  
 YIELD 50%

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



H  
 YIELD 29%

RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)  
 RGT V 10025-87-3 POC13  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT U 62-53-3  
 SOL 64-17-5 EtOH

STAGE(3)  
 RGT W 7647-01-0 HCl  
 SOL 7732-18-5 Water

PRO B 195382-10-6

RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

RX(2) RCT F 1193-02-8, C 160846-41-3

STAGE(1)  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT G 6160-65-2

STAGE(3)  
 SOL 60-29-7 Et2O

STAGE(4)  
 SOL 7732-18-5 Water, 67-56-1 MeOH

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)  
 RGT V 10025-87-3 POC13  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT U 62-53-3  
 SOL 64-17-5 EtOH

STAGE(3)  
 RGT W 7647-01-0 HCl  
 SOL 7732-18-5 Water

PRO B 195382-10-6

RX(1) RCT A 29636-96-2, B 195382-10-6  
 RGT D 127-09-3 AcONa  
 PRO C 160846-41-3  
 SOL 64-17-5 EtOH

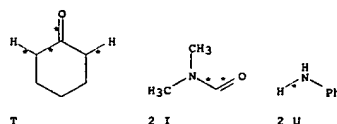
RX(6) RCT F 1193-02-8

STAGE(1)  
 SOL 68-12-2 DMF

STAGE(2)  
 RCT C 160846-41-3

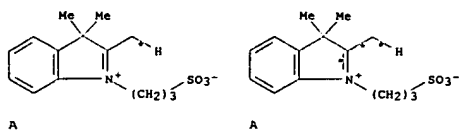
PRO X 195382-11-7

RX(36) OF 44 COMPOSED OF RX(5), RX(1), RX(7)  
 RX(36) T + 2 I + 2 U + 2 A + Y ==> Z

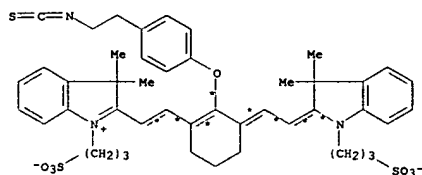


L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



3  
STEPS



YIELD 32%

RX(5) RCT T 108-94-1, I 68-12-2

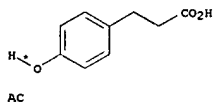
STAGE(1)  
RGT V 10025-87-3 POC13  
SOL 68-12-2 DMF

STAGE(2)  
RCT U 62-53-3  
SOL 64-17-5 EtOH

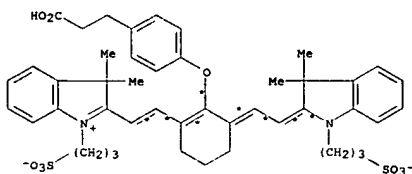
STAGE(3)  
RGT W 7647-01-0 HCl

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



3  
STEPS



YIELD 31%

RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)  
RGT V 10025-87-3 POC13  
SOL 68-12-2 DMF

STAGE(2)  
RCT U 62-53-3  
SOL 64-17-5 EtOH

STAGE(3)  
RGT W 7647-01-0 HCl  
SOL 7732-18-5 Water

PRO B 195382-10-6

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

RX(9) RCT AC 501-97-3

STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3

L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

SOL 7732-18-5 Water

PRO B 195382-10-6

RX(1) RCT A 29636-96-2, B 195382-10-6  
RGT D 127-09-3 AcONa  
PRO C 160846-41-3  
SOL 64-17-5 EtOH

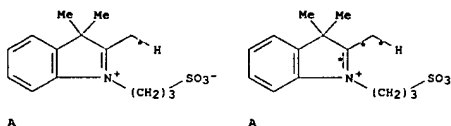
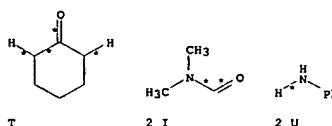
RX(7) RCT Y 60114-04-7

STAGE(1)  
RGT AA 7646-69-7 NaH  
SOL 68-12-2 DMF

STAGE(2)  
RCT C 160846-41-3  
SOL 68-12-2 DMF

PRO Z 195382-08-2

RX(37) OF 44 COMPOSED OF RX(5), RX(1), RX(9)  
RX(37) T + 2 I + 2 U + 2 A + AC ----> M



L2 ANSWER 36 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

PRO M 195382-12-8

L2 ANSWER 37 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 119:28018 CASREACT  
 TITLE: Preparation of indolinispirobenzopyran derivatives  
 INVENTOR(S): Miyashita, Akira  
 PATENT ASSIGNEE(S): Otsuka Kagaku K. K., Japan  
 SOURCE: PCT Int. Appl., 37 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

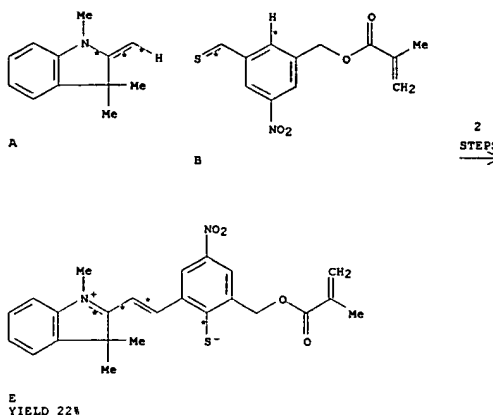
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9216505	A1	19921001	WO 1992-JP292	19920311
W: CA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
JP 04283563	A2	19921008	JP 1991-47203	19910313
JP 3165864	B2	20010514		
EP 529100	A1	19930303	EP 1992-906700	19920311
EP 529100	B1	19981111		
R: DE, FR, GB				
US 5403702	A	19950404	US 1994-230885	19940420
PRIORITY APPLN. INFO.:				
OTHER SOURCE(S): HARPAT 119:28018				
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. [I, II; R1 = C1-20 aralkyl, methacryloxymethyl, methacryloxymethyl; R2-R7 = H, etc.; R8 = H, methacryloxymethyl, etc.; Y = O, S], useful as thermochromic and photochromic materials, are prepared by refluxing a mixture of aldehyde III and indoline derivative IV in MeCOEt gave 73% spiro compound I [R1 = Me, R2-R7 = H, R8 = methacryloxymethyl, Y = S], which was dissolved in MeOH to give a transparent light yellow solution, which was irradiated with 500-W Hg lamp at room temperature to give 22% photomerocyanine form II (R1-R8 and Y remain unchanged) of dark blue crystals. The blue crystals were pulverized and made into a thermochromic recorder sheet to show good contrast.

RX(1) OF 3 COMPOSED OF RX(1), RX(2)  
 RX(3) A + B ==> E

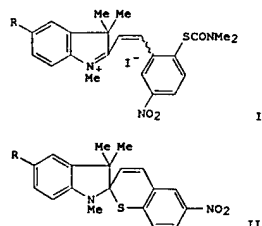
L2 ANSWER 37 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(1) RCT A 118-12-7, B 146966-62-3  
 PRO C 132221-42-2  
 SOL 78-93-3 EtCOMe  
 NTE reflux under N

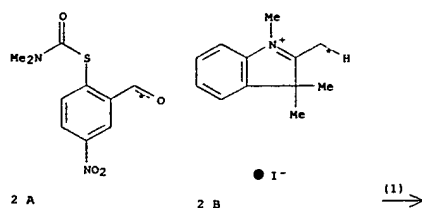
RX(2) RCT C 132221-42-2  
 PRO E 146966-55-4  
 SOL 67-56-1 MeOH  
 NTE photochem., UV

L2 ANSWER 38 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 118:38733 CASREACT  
 TITLE: An improved procedure for the synthesis of indolinispirobenzothioindolopyrans with a nitro group at the 6-position  
 AUTHOR(S): Abe, Yasuo; Gao, Yuan; Nakao, Ren; Horii, Toyokazu; Inoue, Hiroo; Kitao, Teijiro  
 CORPORATE SOURCE: Res. Inst. Adv. Sci. Technol., Univ. Osaka Prefect., Sakai, 593, Japan  
 SOURCE: Chemistry Express (1992), 7(10), 769-72  
 CODEN: CHEXEU; ISSN: 0911-9566  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

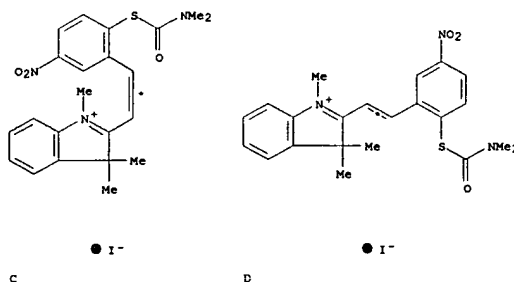


AB Condensation of 1,2,3,3-tetramethylindolium iodides and 5-nitro-2-(N,N-dimethylcarbamoylthio)benzaldehyde gave phenylethenylindoliums I (R = H, NO2) which on hydrolysis underwent spirocyclization to give the title compds. II.

RX(1) OF 5 2 A + 2 B ==> C + D...

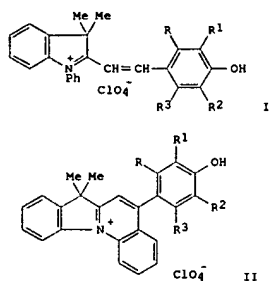


L2 ANSWER 38 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(1) RCT A 145178-02-5, B 5410-63-3  
 RGT E 280-57-9 Triethylenediamine  
 PRO C 145178-03-6, D 145178-04-7  
 SOL 68-12-2 DMF  
 NTE 77% overall

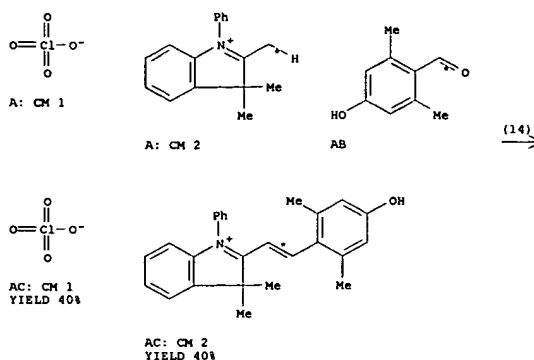
L2 ANSWER 39 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 113:61292 CASREACT  
 TITLE: Photochemistry of hemicyanines. Part III. Synthesis of 5-(hydroxyaryl)-7,7-dimethyl-7H-indolo[1,2-a]quinolinium perchlorates and determination of their acidities  
 AUTHOR(S): Soroka, Krystyna B.; Soroka, Jacek A.  
 CORPORATE SOURCE: Inst. Chem. Eng. Phys. Chem., Tech. Univ. Szczecin, Szczecin, PL-71-065, Pol.  
 SOURCE: Chemica Scripta (1989), 29(2), 167-71  
 CODEN: CSRPB9; ISSN: 0004-2056  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Photochem. and thermal dehydrocyclizations of a series of 1-phenyl-2-[2-(hydroxyaryl)vinyl]-3,3-dimethyl-7H-indolium perchlorates I (R-R3 = H, Me, OMe, halo, etc.) gave title compds. II. I and II dissociate and form deeply colored zwitterions. Spectrophotometrically determined dissociation consts. follow a 2-parameter Taft equation. II are weaker acids than the corresponding I because there is better chance for delocalization of the pos. charge in the quinolinium salts.

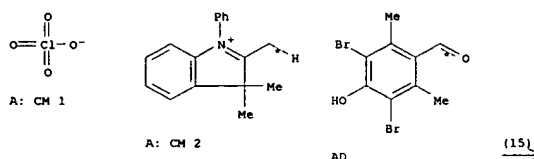
RX(14) OF 56 A + AB ==> AC

L2 ANSWER 39 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

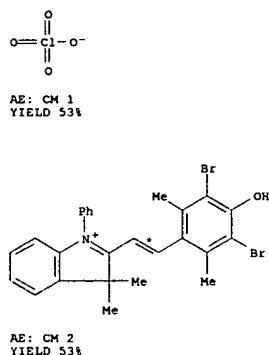


RX(14) RCT A 86879-81-4, AB 70547-87-4  
 PRO AC 128596-40-7

RX(15) OF 56 A + AD ==> AE...

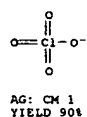
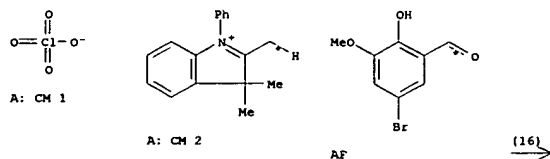


L2 ANSWER 39 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

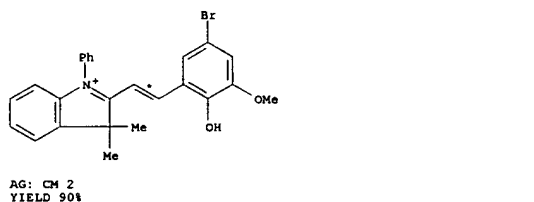


RX(15) RCT A 86879-81-4, AD 128596-79-2  
 PRO AE 128612-05-5

RX(16) OF 56 A + AF ==> AG...

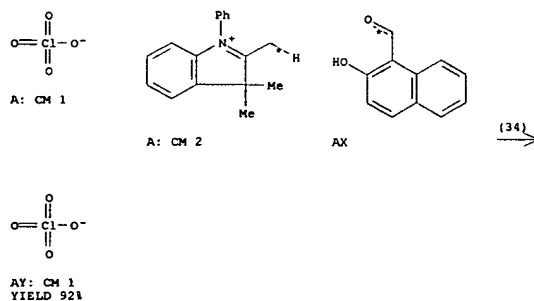


L2 ANSWER 39 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



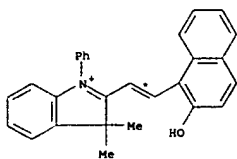
RX(16) RCT A 86879-81-4, AF 5034-74-2  
 PRO AG 128596-44-1

RX(34) OF 56 A + AX ==> AY...



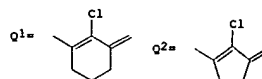
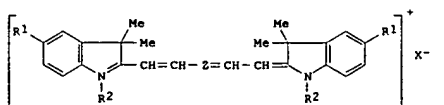


L2 ANSWER 39 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

AY: CH 2  
YIELD 92%RX(34) RCT A 86879-81-4, AX 708-06-5  
PRO AY 128596-46-3

L2 ANSWER 40 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 111:41365 CASREACT  
 TITLE: Indolinecarbocyanine dyes for optical recording materials  
 INVENTOR(S): Psaar, Hubertus; Raue, Roderich  
 PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.  
 SOURCE: Ger. Offen., 8 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

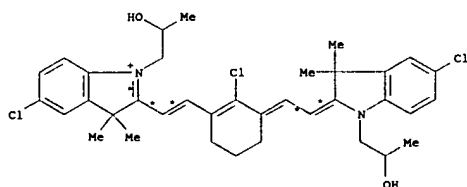
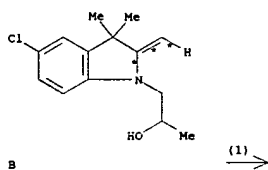
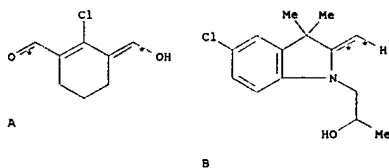
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3721850	A1	19890112	DE 1987-3721850	19870702
PRIORITY APPLN. INFO.: DE 1987-3721850 19870702				
OTHER SOURCE(S): MARPAT 111:41365				



AB Indolinecarbocyanine dyes I (R1 = H, Cl, Cl-4 alkoxy, Cl-4 alkoxy carbonyl, acetoxyl; R2 = (un)substituted alkyl, (un)substituted arylalkyl; X = anion; Z = Q1, Q2), having strong IR absorption, useful in GaAs laser-emissible optical recording materials, are prepared 2-Chloro-1-formyl-3-(hydroxymethylene)cyclohexene was reacted with 1-(hydroxypropyl)-3,3-dimethyl-5-chloro-2-methyleneindoline in Ac2O for 10 h at 50°, and the product washed with 5% aqueous NaCl solution, forming I (R1 = X = Cl, R2 = CH2C(OH)HMe, Z = Q1), λ<sub>max</sub> (MeOH) 788 nm.

RX(1) OF 1 A + 2 B ==&gt; C

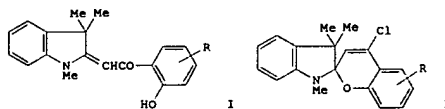
L2 ANSWER 40 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

● Cl<sup>-</sup>

C

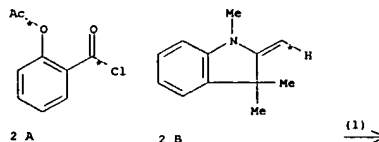
RX(1) RCT A 61010-04-6, B 121263-41-0  
PRO C 121263-42-1

L2 ANSWER 41 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 109:92744 CASREACT  
 TITLE: Synthesis of 4-chloro-substituted spiro[pyran-indolines]  
 AUTHOR(S): Przhivalgovskaya, N. M.; Kon'kov, L. I.; Kurkovskaya, L. N.; Mandzhikov, V. F.  
 CORPORATE SOURCE: Moskv. Khim.-Tekhnol. Inst., Moscow, USSR  
 SOURCE: Khimiya Geterotsiklicheskih Soedinenii (1987), (10), 1346-9  
 CODEN: KGSSAQ; ISSN: 0453-8234  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian



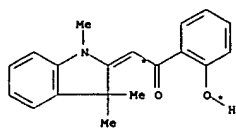
AB [(Hydroxyaroyl)methylene]indolines I (R = H, 3-Me, 5-NO<sub>2</sub>, etc.), prepared from 1,3,3-trimethyl-2-methyleneindoline and o-acetoxyaroyl chlorides, when heated with POCl<sub>3</sub> and then treated with alkali, gave spiro[chlorobenzopyran-indolines] II, which, in contrast to unsubstituted analogs, do not have photochromic properties.

RX(1) OF 21 ...2 A + 2 B ==&gt; C + D...

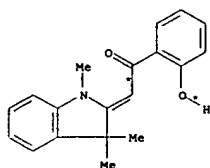


(1) →

L2 ANSWER 41 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



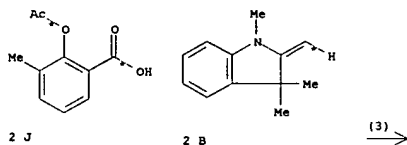
C



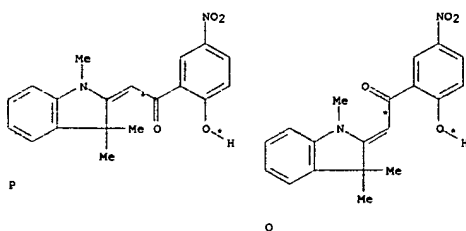
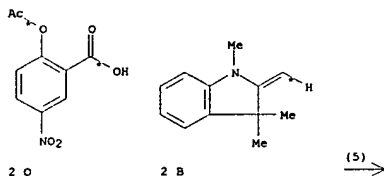
D

RX(1) RCT A 5538-51-2, B 118-12-7  
 RGT E 121-44-8 Et3N  
 PRO C 115978-91-1, D 115978-92-2  
 SOL 71-43-2 Benzene  
 NTE 73% Overall

RX(3) OF 21 2 J + 2 B ==&gt; K + L...



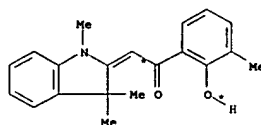
L2 ANSWER 41 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



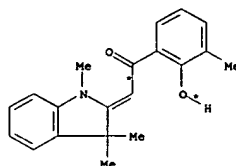
RX(5) RCT O 17336-14-0  
 STAGE(1)  
 RGT M 7719-09-7 SOC12  
 SOL 71-43-2 Benzene  
 STAGE(2)  
 RCT B 118-12-7  
 RGT E 121-44-8 Et3N  
 SOL 71-43-2 Benzene  
 PRO P 115978-95-5, Q 115978-96-6  
 NTE 80% Overall

RX(7) OF 21 2 S + 2 B ==&gt; T + U...

L2 ANSWER 41 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



K

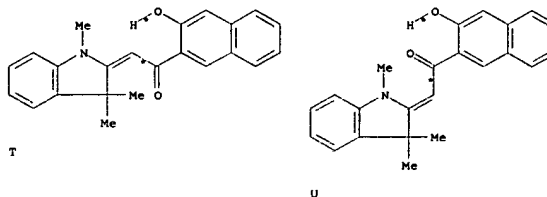
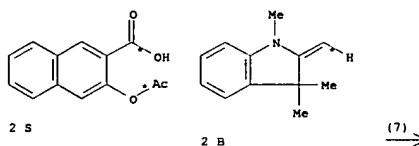


L

RX(3) RCT J 4386-39-4  
 STAGE(1)  
 RGT M 7719-09-7 SOC12  
 SOL 71-43-2 Benzene  
 STAGE(2)  
 RCT B 118-12-7  
 RGT E 121-44-8 Et3N  
 SOL 71-43-2 Benzene  
 PRO K 115978-93-3, L 115978-94-4  
 NTE 32% Overall

RX(5) OF 21 2 O + 2 B ==&gt; P + Q...

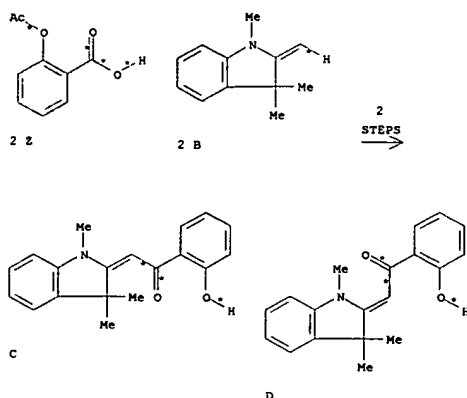
L2 ANSWER 41 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(7) RCT S 5464-07-3  
 STAGE(1)  
 RGT M 7719-09-7 SOC12  
 SOL 71-43-2 Benzene  
 STAGE(2)  
 RCT B 118-12-7  
 RGT E 121-44-8 Et3N  
 SOL 71-43-2 Benzene  
 PRO T 115978-97-7, U 115978-98-8  
 NTE 43% Overall

RX(18) OF 21 COMPOSED OF RX(11), RX(1)  
 RX(18) 2 Z + 2 B ==> C + D

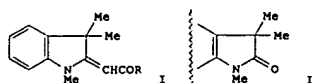
L2 ANSWER 41 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(11) RCT Z 50-78-2  
 RGT M 7719-09-7 SOC12  
 PRO A 5538-51-2  
 SOL 71-43-2 Benzene

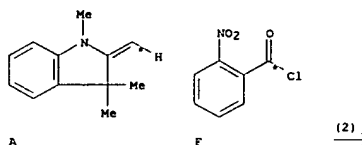
RX(1) RCT A 5538-51-2, B 118-12-7  
 RGT E 121-44-8 Et3N  
 PRO C 115978-91-1, D 115978-92-2  
 SOL 71-43-2 Benzene  
 NTE 73% Overall

L2 ANSWER 42 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
 108:150216 CASREACT  
 TITLE: Acetylenic fragmentation of acylated derivatives of Fischer's base.  
 AUTHOR(S): Przhiyalgovskaya, N. M.; Kon'kov, L. I.; Tarshits, D. L.; Salmina, S. V.; Segizova, N. T.; Suvorov, N. N.  
 CORPORATE SOURCE: Mosk. Khim.-Tekhnol. Inst., Moscow, USSR  
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1987), (7), 915-18  
 CODEN: KGSSAQ; ISSN: 0453-8234  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 GI

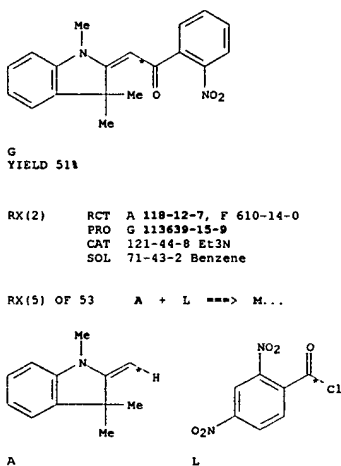


AB Acylation of Fischer's base by  $\text{RCOCl}$  ( $\text{R} = \text{alkyl, aryl, hetaryl}$ ) gave 31-84% indolines I (18 compds.) which were cleaved by  $\text{POCl}_3\text{-NaOH}$  to give 48-87% oxindole II and 35-87%  $\text{RC.tplbond.CH}$  ( $\text{R} = \text{aryl}$ ).

RX(2) OF 53 A + F ==&gt; G...

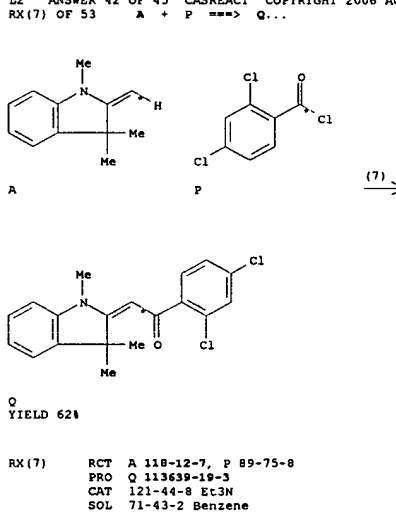


L2 ANSWER 42 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



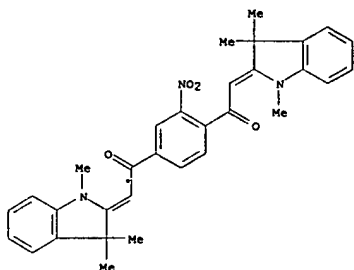
RX(5) RCT A 118-12-7, L 20195-22-6  
 PRO M 113639-17-1  
 CAT 121-44-8 Et3N  
 SOL 71-43-2 Benzene

L2 ANSWER 42 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L2 ANSWER 42 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

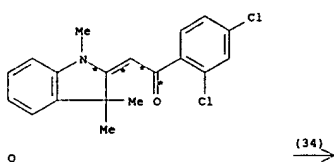
(Continued)



AA  
YIELD 75%

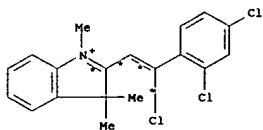
RX(12) RCT A 118-12-7, 2 113639-29-5  
PRO AA 113639-22-8  
CAT 121-44-8 Et3N  
SOL 71-43-2 Benzene

RX(34) OF 53 ...Q ==> BG...



L2 ANSWER 42 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)



● Cl<sup>-</sup>

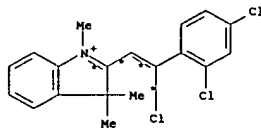
BG  
YIELD 90%

RX(7) RCT A 118-12-7, P 89-75-8  
PRO Q 113639-19-3  
CAT 121-44-8 Et3N  
SOL 71-43-2 Benzene

RX(34) RCT Q 113639-19-3  
RGT AP 10025-87-3 POC13  
PRO BG 113655-34-8  
SOL 109-99-9 THF

L2 ANSWER 42 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

(Continued)

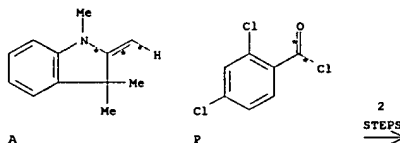


● Cl<sup>-</sup>

BG  
YIELD 90%

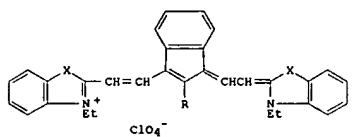
RX(34) RCT Q 113639-19-3  
RGT AP 10025-87-3 POC13  
PRO BG 113655-34-8  
SOL 109-99-9 THF

RX(43) OF 53 COMPOSED OF RX(7), RX(34)  
RX(43) A + P ==> BG



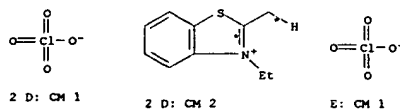
L2 ANSWER 43 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 100:53180 CASREACT  
TITLE: Synthesis of meso-substituted tricarboquinone dyes with an o-phenylene bridge in the chromophore  
AUTHOR(S): Sosnovskii, G. M.; Lugovskii, A. P.; Tishchenko, I. G.  
CORPORATE SOURCE: Beloruss. Gos. Univ., Minsk, USSR  
SOURCE: Zhurnal Organicheskoi Khimii (1983), 19(10), 2143-6  
CODEN: ZORKAE; ISSN: 0514-7492  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
GI

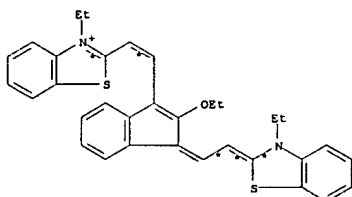
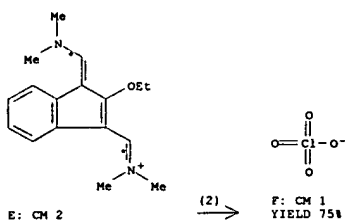


AB The phenylene-bridged tricarboquinones I (R = OEt, Ph; X = S, CH:CH, CHMeEt) and an analogous 4,4'-quinotricarboquinone absorb at lower wavelength than the resp. ethylene-bridged compds. by 70-100 nm. 2-Indanone (II) [615-13-4] was converted to the enol ether with HC(OEt)3, bis-aminoformylated with DMF-POC13, and condensed with heterocyclic quaternary compds. to give two I (R = OEt) and the analog. II was treated with PhMgBr, condensed with Me2NCH(OMe)2, aminoformylated, and condensed with heterocyclic quaternary compds. to give the remaining three I. The I are luminescent with a low quantum yield (10-15%).

RX(2) OF 16 2 D + E ==> F

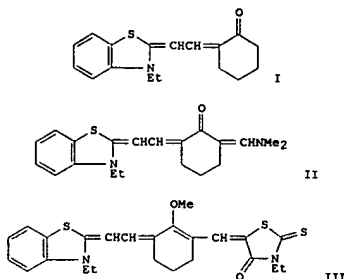


L2 ANSWER 43 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

F: CM 2  
YIELD 75%RX(2) RCT D 50378-73-9, E 88505-12-8  
PRO F 88505-00-4

L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN

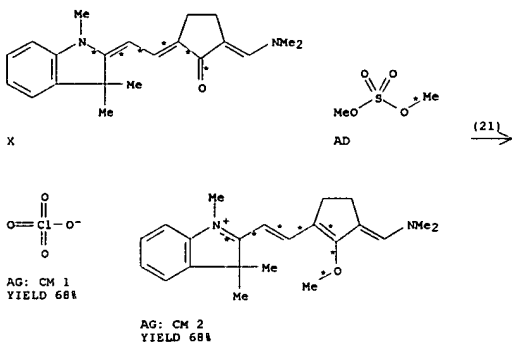
100:35826 CASREACT  
TITLE: Polymethine dyes with hydrocarbon bridges. Enamine ketones in the chemistry of cyanine dyes  
AUTHOR(S): Slominskii, Yu. L.; Radchenko, I. D.; Popov, S. V.; Tolmachev, A. I.  
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR  
SOURCE: Zhurnal Organicheskoi Khimii (1983), 19(10), 2134-42  
DOCUMENT TYPE: CODEN: ZORKAE; ISSN: 0514-7492  
LANGUAGE: Russian  
GI



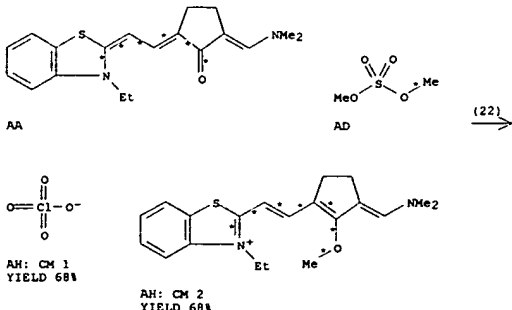
AB Cyclopentanone [120-92-3] and cyclohexanone [108-94-1] react with Me<sub>2</sub>NCH(OMe)<sub>2</sub> [4637-24-5] to give the mono- and bis(enamine) ketones, which are useful in the synthesis of merocyanines and cyanines with bridging groups. For example, 2-(dimethylaminomethylene)cyclohexanone [6135-19-9] reacted with 3-ethyl-2-methylbenzothiazolium p-toluenesulfonate [14933-76-7] in boiling pyridine to give I [88340-49-2] in 87% yield and with 2-(dimethylaminovinyl)-3-ethylbenzothiazolium iodide [17579-01-0] in pyridine containing NaOMe to give II [88340-50-5] in 71% yield. O-Methylation of II, reaction with PhNH<sub>2</sub>, and condensation with N-ethylrhodanine [7648-01-3] gave III [88340-51-6] in 26% yield, based on II. 1H NMR studies showed that I and II, as well as their cyclopentanone analogs, have a pseudo-trans configuration.

RX(21) OF 79 ...X + AD ==&gt; AG

L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(21) RCT X 88340-85-6, AD 77-78-1  
PRO AG 88340-73-2

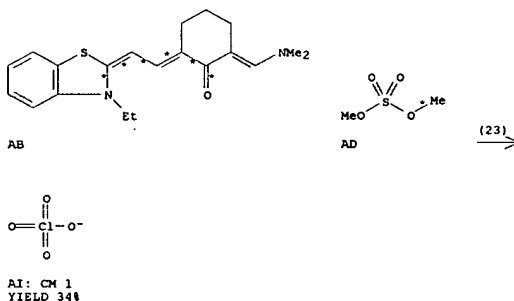
RX(22) OF 79 ...AA + AD ==&gt; AH...



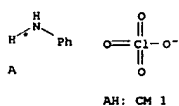
L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(22) RCT AA 88340-84-5, AD 77-78-1  
PRO AH 88340-75-4

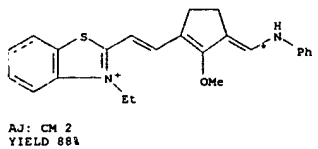
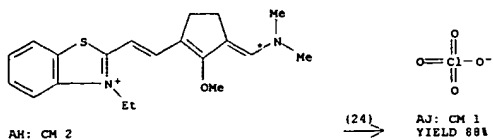
RX(23) OF 79 ...AB + AD ==&gt; AI...

RX(23) RCT AB 88340-50-5, AD 77-78-1  
PRO AI 88340-77-6

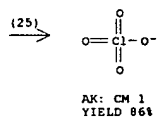
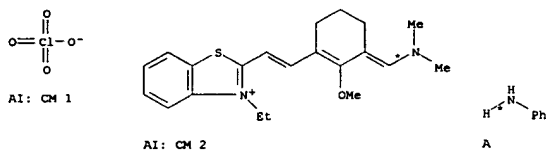
RX(24) OF 79 ...A + AH ==&gt; AJ...



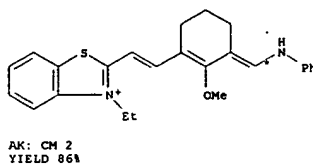
L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(24) RCT A 62-53-3, AH 88340-75-4  
PRO AJ 88340-79-8

RX(25) OF 79 ...AJ + A ==&gt; AK...



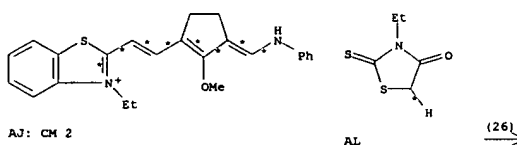
L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(25) RCT AI 88340-77-6, A 62-53-3  
PRO AK 88340-81-2

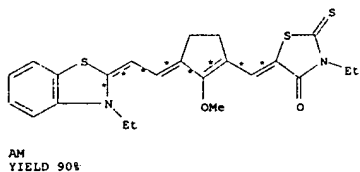
RX(26) OF 79 ...AJ + AL ==&gt; AM



AJ: CM 1



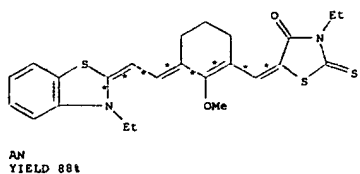
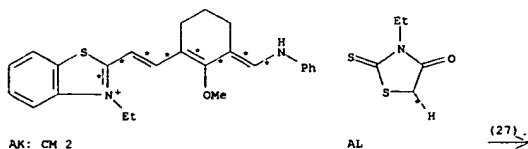
L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(26) RCT AJ 88340-79-8, AL 7648-01-3  
PRO AM 88340-82-3

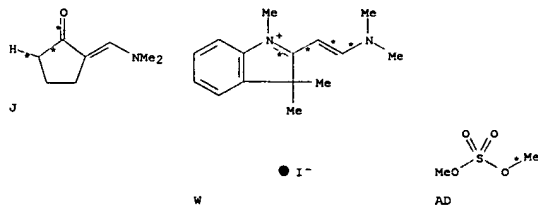
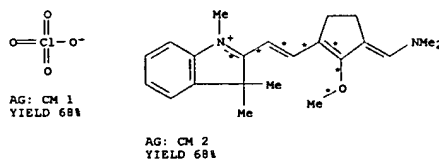
RX(27) OF 79 ...AK + AL ==&gt; AN



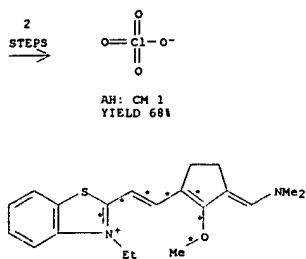
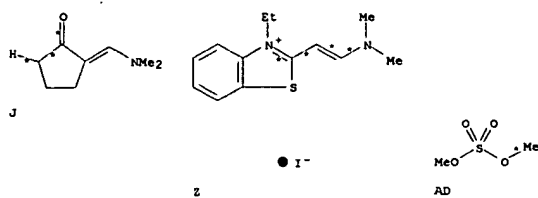
AK: CM 1



L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(27) RCT AK 88340-81-2, AL 7648-01-3  
PRO AN 88340-51-6RX(50) OF 79 COMPOSED OF RX(14), RX(21)  
RX(50) J + W + AD ==> AG2  
STEPSRX(14) RCT J 62041-55-8, W 53704-27-1  
PRO X 88340-85-6RX(21) RCT X 88340-85-6, AD 77-78-1  
PRO AG 88340-73-2RX(51) OF 79 COMPOSED OF RX(16), RX(22)  
RX(51) J + E + AD ==> AH

L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

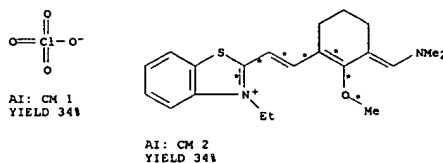
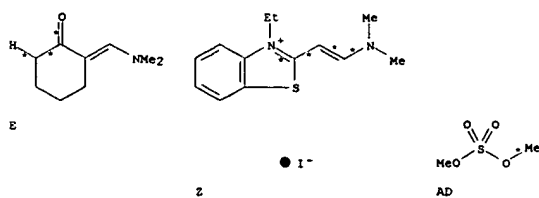


RX(16) RCT J 62041-55-8, Z 17579-01-0  
PRO AA 88340-84-5

RX(22) RCT AA 88340-84-5, AD 77-78-1  
PRO AH 88340-75-4

RX(52) OF 79 COMPOSED OF RX(17), RX(23)  
RX(52) E + Z + AD ==> AI

L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

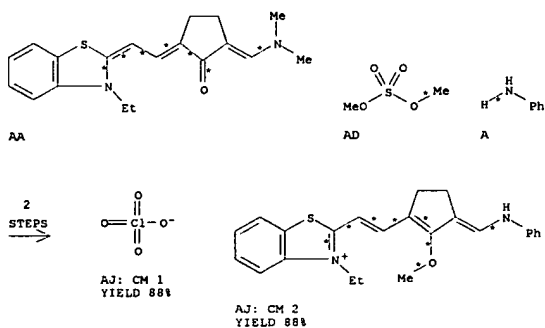


RX(17) RCT E 6135-19-9, Z 17579-01-0  
PRO AB 88340-50-5

RX(23) RCT AB 88340-50-5, AD 77-78-1  
PRO AI 88340-77-6

RX(53) OF 79 COMPOSED OF RX(22), RX(24)  
RX(53) AA + AD + A ==> AJ

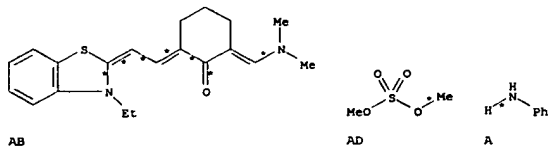
L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



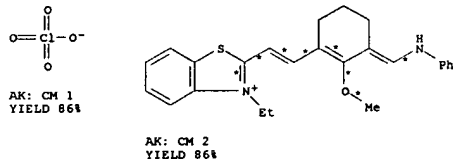
RX(22) RCT AA 88340-84-5, AD 77-78-1  
PRO AH 88340-75-4

RX(24) RCT A 62-53-3, AH 88340-75-4  
PRO AJ 88340-79-8

RX(54) OF 79 COMPOSED OF RX(23), RX(25)  
RX(54) AB + AD + A ==> AK



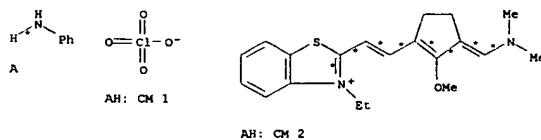
L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



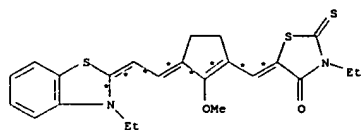
RX(23) RCT AB 88340-50-5, AD 77-78-1  
PRO AI 88340-77-6

RX(25) RCT AI 88340-77-6, A 62-53-3  
PRO AK 88340-81-2

RX(55) OF 79 COMPOSED OF RX(24), RX(26)  
RX(55) A + AH + AL ==> AM



L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

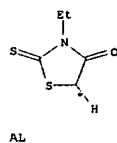
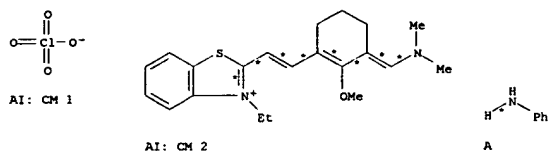


AM  
YIELD 90%

RX(24) RCT A 62-53-3, AH 88340-75-4  
PRO AJ 88340-79-8

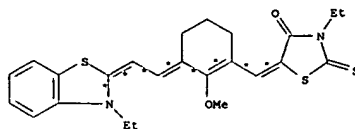
RX(26) RCT AJ 88340-79-8, AL 7648-01-3  
PRO AH 88340-82-3

RX(56) OF 79 COMPOSED OF RX(25), RX(27)  
RX(56) AI + A + AL ==> AN



2  
STEPS

L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

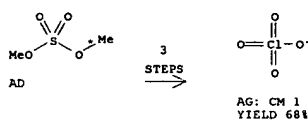
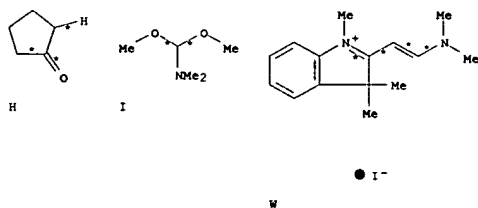


AN  
YIELD 88%

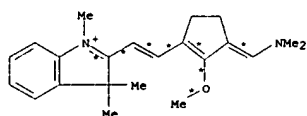
RX(25) RCT AI 88340-77-6, A 62-53-3  
PRO AK 88340-81-2

RX(27) RCT AK 88340-81-2, AL 7648-01-3  
PRO AN 88340-51-6

RX(63) OF 79 COMPOSED OF RX(3), RX(14), RX(21)  
RX(63) H + I + W + AD ==> AG



L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



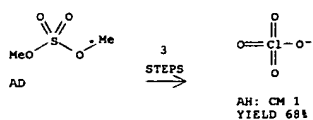
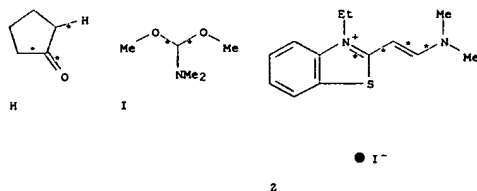
AG: CM 2  
YIELD 68%

RX(3) RCT H 120-92-3, I 4637-24-5  
PRO J 62041-55-8

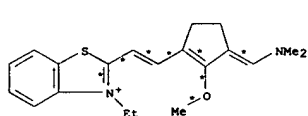
RX(14) RCT J 62041-55-8, W 53704-27-1  
PRO X 88340-85-6

RX(21) RCT X 88340-85-6, AD 77-78-1  
PRO AG 88340-73-2

RX(64) OF 79 COMPOSED OF RX(3), RX(16), RX(22)  
RX(64) H + I + Z + AD ==> AH



L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



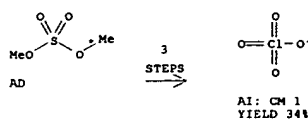
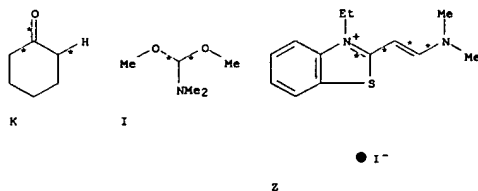
AH: CM 2  
YIELD 68%

RX(3) RCT H 120-92-3, I 4637-24-5  
PRO J 62041-55-8

RX(16) RCT J 62041-55-8, Z 17579-01-0  
PRO AA 88340-84-5

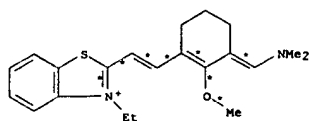
RX(22) RCT AA 88340-84-5, AD 77-78-1  
PRO AH 88340-75-4

RX(67) OF 79 COMPOSED OF RX(4), RX(17), RX(23)  
RX(67) K + I + Z + AD ==> AI





L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



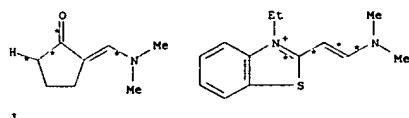
AI: CM 2  
YIELD 34%

RX(4) RCT K 108-94-1, I 4637-24-5  
PRO E 6135-19-9

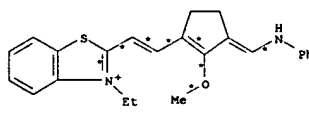
RX(17) RCT E 6135-19-9, Z 17579-01-0  
PRO AB 88340-50-5

RX(23) RCT AB 88340-50-5, AD 77-78-1  
PRO AI 88340-77-6

RX(70) OF 79 COMPOSED OF RX(16), RX(22), RX(24)  
RX(70) J + E + AD + A ==> AJ



L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



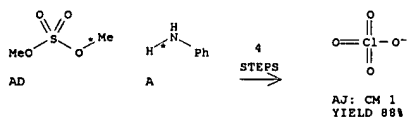
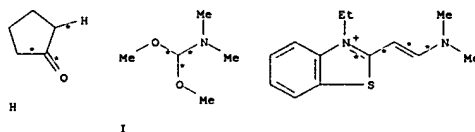
AJ: CM 2  
YIELD 88%

RX(16) RCT J 62041-55-8, Z 17579-01-0  
PRO AA 88340-84-5

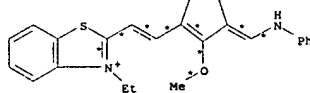
RX(22) RCT AA 88340-84-5, AD 77-78-1  
PRO AH 88340-75-4

RX(24) RCT A 62-53-3, AH 88340-75-4  
PRO AJ 88340-79-8

RX(71) OF 79 COMPOSED OF RX(3), RX(16), RX(22), RX(24)  
RX(71) H + I + E + AD + A ==> AJ



L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



AJ: CM 2  
YIELD 88%

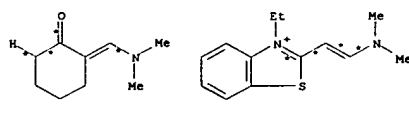
RX(3) RCT H 120-92-3, I 4637-24-5  
PRO J 62041-55-8

RX(16) RCT J 62041-55-8, Z 17579-01-0  
PRO AA 88340-84-5

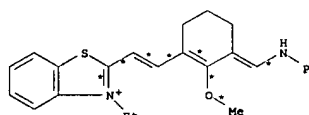
RX(22) RCT AA 88340-84-5, AD 77-78-1  
PRO AH 88340-75-4

RX(24) RCT A 62-53-3, AH 88340-75-4  
PRO AJ 88340-79-8

RX(72) OF 79 COMPOSED OF RX(17), RX(23), RX(25)  
RX(72) E + E + AD + A ==> AK



L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



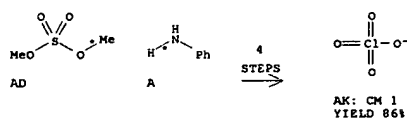
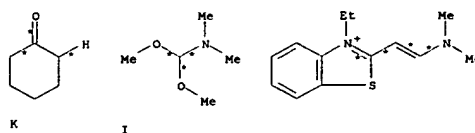
AK: CM 2  
YIELD 86%

RX(17) RCT E 6135-19-9, Z 17579-01-0  
PRO AB 88340-50-5

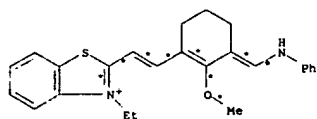
RX(23) RCT AB 88340-50-5, AD 77-78-1  
PRO AI 88340-77-6

RX(25) RCT AI 88340-77-6, A 62-53-3  
PRO AK 88340-81-2

RX(73) OF 79 COMPOSED OF RX(4), RX(17), RX(23), RX(25)  
RX(73) K + I + E + AD + A ==> AK

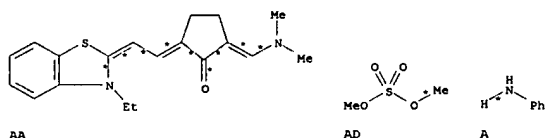


L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

AK: CM 2  
YIELD 86%RX(4) RCT K 108-94-1, I 4637-24-5  
PRO E 6135-19-9RX(17) RCT E 6135-19-9, Z 17579-01-0  
PRO AB 88340-50-5RX(23) RCT AB 88340-50-5, AD 77-78-1  
PRO AI 88340-77-6RX(25) RCT AI 88340-77-6, A 62-53-3  
PRO AK 88340-81-2

RX(74) OF 79 COMPOSED OF RX(22), RX(24), RX(26)

RX(74) AA + AD + A + AL ==&gt; AM

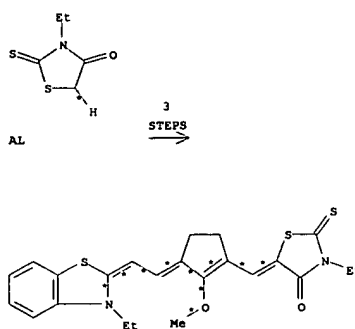


AA

AD

A

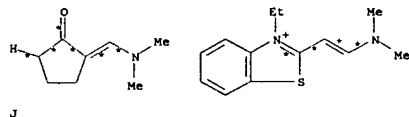
L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

AM  
YIELD 90%RX(22) RCT AA 88340-84-5, AD 77-78-1  
PRO AH 88340-75-4RX(24) RCT A 62-53-3, AH 88340-75-4  
PRO AJ 88340-79-8RX(26) RCT AJ 88340-79-8, AL 7648-01-3  
PRO AM 88340-82-3

RX(75) OF 79 COMPOSED OF RX(16), RX(22), RX(24), RX(26)

RX(75) J + Z + AD + A + AL ==&gt; AM

L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

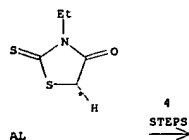


J

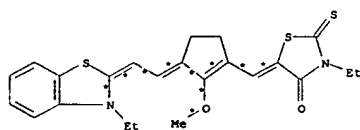
Z



A



AL

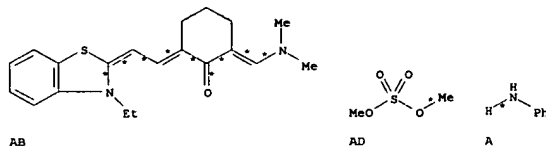
4  
STEPSAM  
YIELD 90%RX(16) RCT J 62041-55-8, Z 17579-01-0  
PRO AA 88340-84-5RX(22) RCT AA 88340-84-5, AD 77-78-1  
PRO AH 88340-75-4

L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(24) RCT A 62-53-3, AH 88340-75-4  
PRO AJ 88340-79-8RX(26) RCT AJ 88340-79-8, AL 7648-01-3  
PRO AM 88340-82-3

RX(76) OF 79 COMPOSED OF RX(23), RX(25), RX(27)

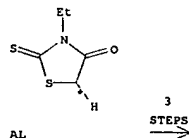
RX(76) AB + AD + A + AL ==&gt; AM



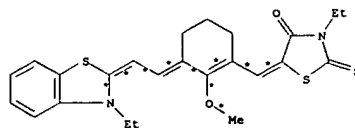
AB

AD

A

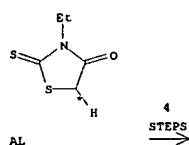
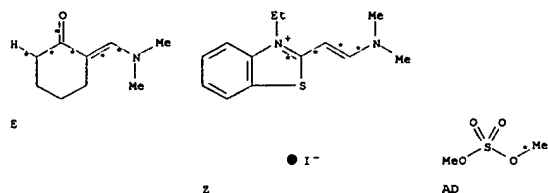


AL

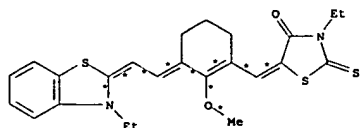
3  
STEPSAM  
YIELD 88%RX(23) RCT AB 88340-50-5, AD 77-78-1  
PRO AI 88340-77-6RX(25) RCT AI 88340-77-6, A 62-53-3  
PRO AK 88340-81-2

L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)  
 RX(27) RCT AK 88340-81-2, AL 7648-01-3  
 PRO AN 88340-51-6

RX(77) OF 79 COMPOSED OF RX(17), RX(23), RX(25), RX(27)  
 RX(77) E + Z + AD + A + AL ==> AN



L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



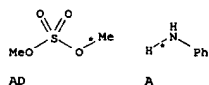
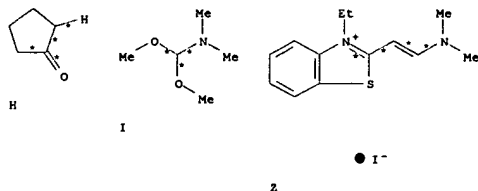
RX(17) RCT E 6135-19-9, Z 17579-01-0  
 PRO AB 88340-50-5

RX(23) RCT AB 88340-50-5, AD 77-78-1  
 PRO AI 88340-77-6

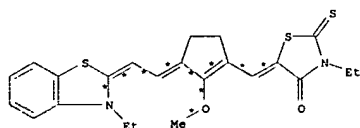
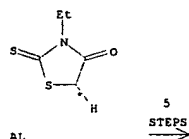
RX(25) RCT AI 88340-77-6, A 62-53-3  
 PRO AK 88340-81-2

RX(27) RCT AK 88340-81-2, AL 7648-01-3  
 PRO AN 88340-51-6

RX(78) OF 79 COMPOSED OF RX(3), RX(16), RX(22), RX(24), RX(26)  
 RX(78) H + I + S + AD + A + AL ==> AN



L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(3) RCT H 120-92-3, I 4637-24-5  
 PRO J 62041-55-8

RX(16) RCT J 62041-55-8, Z 17579-01-0  
 PRO AA 88340-84-5

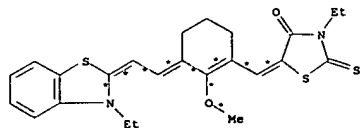
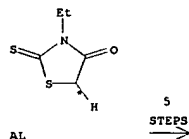
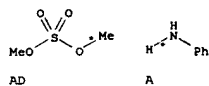
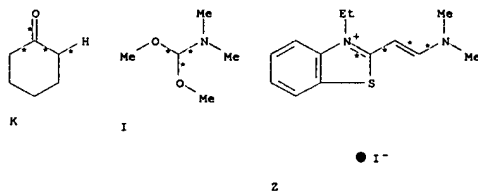
RX(22) RCT AA 88340-84-5, AD 77-78-1  
 PRO AH 88340-75-4

RX(24) RCT A 62-53-3, AH 88340-75-4  
 PRO AJ 88340-79-8

RX(26) RCT AJ 88340-79-8, AL 7648-01-3  
 PRO AM 88340-82-3

RX(79) OF 79 COMPOSED OF RX(4), RX(17), RX(23), RX(25), RX(27)  
 RX(79) K + I + Z + AD + A + AL ==> AN

L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(4) RCT K 108-94-1, I 4637-24-5  
 PRO E 6135-19-9

RX(17) RCT E 6135-19-9, Z 17579-01-0

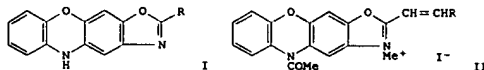
L2 ANSWER 44 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(23) RCT AB 88340-50-5, AD 77-78-1  
PRO AI 88340-77-6

RX(25) RCT AI 88340-77-6, A 62-53-3  
PRO AK 88340-81-2

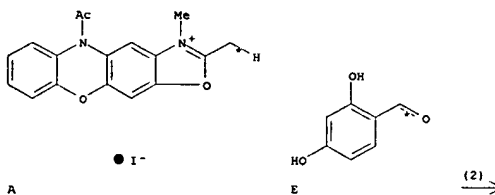
RX(27) RCT AK 88340-81-2, AL 7646-01-3  
PRO AN 88340-51-6

L2 ANSWER 45 OF 45 CASREACT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 84:121744 CASREACT  
TITLE: Heterocyclic compounds. VIII. Studies on  
oxazolophenoxazines  
AUTHOR(S): Osman, A. M.; Metwally, S. A. M.; Youssef, M. S. K.  
CORPORATE SOURCE: Dep. Chem., Assiut Univ., Assiut, Egypt  
SOURCE: Canadian Journal of Chemistry (1976), 54(1), 37-43  
CODEN: CJCHAG; ISSN: 0008-4042  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



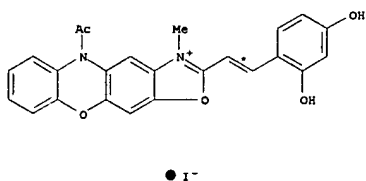
AB 5H-oxazolo[4,5-b]phenoxazine (I, R = H) was synthesized by the reaction of 3-amino-2-hydroxyphenoxazine-HCl with HCHO. The styryloxazolophenoxazines II (R = Ph, m-ClC<sub>6</sub>H<sub>4</sub>, m-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, etc.) were prepared by condensation of 2-methyl-5-acetyloxazolo[4,5-b]phenoxazine methiodide with aromatic aldehydes. The 2-aryl-oxazolophenoxazines I (R = Ph, o-ClC<sub>6</sub>H<sub>4</sub>, o-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, etc.) were synthesized by reaction of 3-aminophenoxaz-2-one with the appropriate aldehydes in the presence of an acid-base catalyst. At 10-3M I (R = o-MeOC<sub>6</sub>H<sub>4</sub>) was bactericidal and fungicidal.

RX(2) OF 2 A + E ==> F



X

L2 ANSWER 45 OF 45 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



F

RX(2) RCT A 59225-25-1, E 95-01-2  
RGT D 7646-85-7 ZnCl<sub>2</sub>  
PRO F 59225-34-2